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* * * * * Welcome to STN International * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAPLUS Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAPLUS updated with revised CAS roles
NEWS 7	JAN 22	CA/CAPLUS enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAPLUS enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAPLUS Indian patent publication number format defined
NEWS 30	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 31	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 32	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 33	MAY 21	CA/CAPLUS enhanced with additional kind codes for German patents
NEWS 34	MAY 22	CA/CAPLUS enhanced with IPC reclassification in Japanese patents
NEWS EXPRESS	NOVEMBER 10	CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS		STN Operating Hours Plus Help Desk Availability

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 13:01:54 ON 22 MAY 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 21 MAY 2007 HIGHEST RN 935505-97-8
DICTIONARY FILE UPDATES: 21 MAY 2007 HIGHEST RN 935505-97-8

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

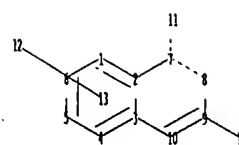
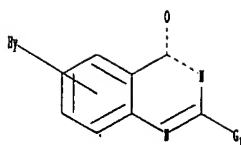
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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Uploading C:\Program Files\Stnexp\Queries\10530897.str



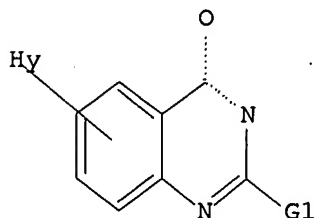
chain nodes :
 11 12 14
 ring nodes :
 1 2 3 4 5 6 7 8 9 10
 chain bonds :
 7-11 9-14
 ring bonds :
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 exact/norm bonds :
 2-7 3-10 7-8 7-11 8-9 9-10 9-14
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 isolated ring systems :
 containing 1 :

G1:C,O,N

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:CLASS 12:Atom 13:Atom 14:CLASS
 Element Count :
 Node 12: Limited
 C,C3-7
 O,O0-2
 N,N0-1

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=> d L1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:02:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 19385 TO ITERATE

10.3% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 379364 TO 396036
PROJECTED ANSWERS: 7 TO 379

L2 1 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 13:02:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 387895 TO ITERATE

100.0% PROCESSED 387895 ITERATIONS 484 ANSWERS
SEARCH TIME: 00.00.13

L3 484 SEA SSS FUL L1

=> file zcaplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
	172.55	172.76

FILE 'ZCAPLUS' ENTERED AT 13:03:18 ON 22 MAY 2007
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FILE COVERS 1907 - 22 May 2007 VOL 146 ISS 22
FILE LAST UPDATED: 21 May 2007 (20070521/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 74 L3

=> d his

(FILE 'HOME' ENTERED AT 13:01:54 ON 22 MAY 2007)

FILE 'REGISTRY' ENTERED AT 13:02:14 ON 22 MAY 2007

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 484 S L1 FUL

FILE 'ZCAPLUS' ENTERED AT 13:03:18 ON 22 MAY 2007

L4 74 S L3

=> s l4 1- ibib abs hitstr

MISSING OPERATOR L4 1-

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> d l4 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 74 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:216840 ZCAPLUS

DOCUMENT NUMBER: 146:374365

TITLE: How Do Size-Expanded DNA Nucleobases Enhance Duplex Stability? Computational Analysis of the Hydrogen-Bonding and Stacking Ability of xDNA Bases

AUTHOR(S): McConnell, Tom L.; Wetmore, Stacey D.

CORPORATE SOURCE: Department of Chemistry, Mount Allison University, Sackville, NB, E4L 1G8, Can.

SOURCE: Journal of Physical Chemistry B (2007), 111(11), 2999-3009

CODEN: JPCBFK; ISSN: 1520-6106

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Computational chemical (B3LYP, MP2) is used to study the properties of size-expanded DNA nucleobases generated by inserting a benzene spacer into the natural nucleobases. Although the addition of the spacer does not significantly affect the hydrogen-bonding properties of natural nucleobases, the orientation of the base about the glycosidic bond necessary for Watson-Crick binding is destabilized, which could have implications for the selectivity of expanded bases, as well as the stability of expanded duplexes. Consideration of the (stacked) binding energies in the preferred relative orientation of natural and expanded nucleobases aligned according to their centers of mass reveals that the stacking within natural dimers can be increased by up to 50% upon expansion of one nucleobase and up to 90% upon expansion of two

nucleobases. The implications of these findings to the stability of expanded duplexes were revealed by considering simplified models of natural and mixed duplexes composed of four nucleobases. Although intra- and interstrand interactions within double helixes are typically less than those predicted when nucleobases are stacked according to their centers of mass, some nucleobases utilize their full stacking potential within double helixes, where both intra- and interstrand interactions can be significant. Most importantly, increasing the size of nucleobases within the duplex significantly increases both intra- and interstrand stacking interactions. Specifically, some interactions are double the magnitude of the corresponding intrastrand interactions in natural helixes, and even greater increases in interstrand interactions are sometimes found. Thus, our work suggests that mixed duplexes composed of natural bases hydrogen bound to expanded bases may exploit the increase in the inherent stacking ability of the expanded bases in more than one way and thereby afford duplexes with greater stability than natural DNA.

IT 639465-38-6

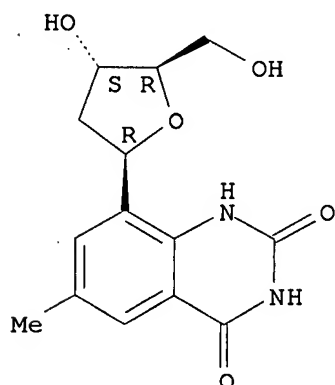
RL: PRP (Properties)

(computational anal. of hydrogen-bonding and stacking ability of size-expanded DNA nucleobases with regard to duplex stability)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-6-one, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

94

THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:146833 ZCAPLUS

DOCUMENT NUMBER: 146:229356

TITLE: Nitric oxide enhancing angiotensin II antagonist compounds, and their preparation, compositions, and methods of use

INVENTOR(S): Garvey, David S.; Cai, Xiong; Fang, Xinqin; Ranatunge, Ramani R.; Wey, Shiow-Jyi; Zhai, Hai-Xiao

PATENT ASSIGNEE(S): Nitromed, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 58pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

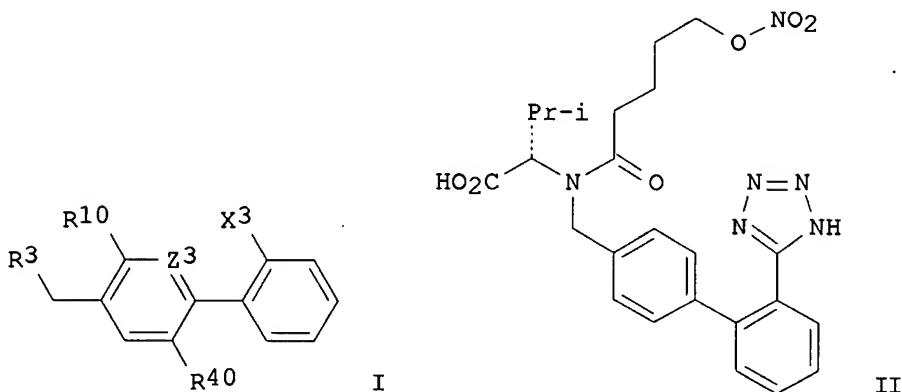
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2007032533	A1	20070208	US 2006-499770	20060807
WO 2007019448	A2	20070215	WO 2006-US30733	20060807
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.:

US 2005-706005P P 20050808
US 2005-706419P P 20050809
US 2005-748579P P 20051209

OTHER SOURCE(S): MARPAT 146:229356
GI



AB The invention describes compns. and kits comprising at least one nitric oxide enhancing angiotensin II antagonist compound of formula I, or pharmaceutically acceptable salts thereof, and compns. comprising at least one nitric oxide enhancing angiotensin II antagonist compound, and, optionally, at least one nitric oxide enhancing compound and/or at least one therapeutic agent. Compds. of formula I wherein X³ is (un)substituted azole, (un)substituted sulfonylaminooxazole, (un)substituted aminosulfonyl, (un)substituted acyl, etc.; Y³ is (un)substituted azole, (un)substitute valine derivative, (un)substituted amide, etc.; Z³ is CH and N; R¹⁰ is F and H; R⁴⁰ is H, lower alkyl, alkoxyalkyl, etc.; and their pharmaceutically acceptable salts thereof are claimed. The invention also provides methods for (a) treating cardiovascular diseases; (b) treating renovascular diseases; (c) treating diabetes; (d) treating diseases resulting from oxidative stress; (e) treating endothelial dysfunctions; (f) treating diseases caused by endothelial dysfunctions; (g) treating cirrhosis; (h) treating pre-eclampsia; (j) treating osteoporosis; (k) treating nephropathy; (l) treating peripheral vascular diseases; (m) treating portal hypertension (o) treating central nervous system disorders; (p) treating metabolic syndrome; and (q) treating hyperlipidemia. The nitric oxide enhancing angiotensin II antagonist compds. comprise at least one nitric oxide enhancing group linked to the angiotensin II antagonist

compound through one or more sites such as carbon, oxygen and/or nitrogen via a bond or moiety that cannot be hydrolyzed. Example compound II was prepared by reduction of 2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-carboxylic acid Me ester; the resulting 2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-methanol underwent oxidation to give 2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-carboxaldehyde, which underwent condensation with L-valine tert-Bu ester hydrochloride to give (E)-N-[2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-methylene]-L-valine tert-Bu ester, which underwent reduction to give N-[2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-methyl]-L-valine tert-Bu ester, which underwent amidation with 5-(nitrooxy)pentanoic acid to give N-[2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-methyl]-N-[5-(nitrooxy)-1-oxopentyl]-L-valine tert-Bu ester, which underwent hydrolysis to give N-[2'[2-(1-methyl-1-phenylethyl)-2H-tetrazol-5-yl]-[1,1'-biphenyl]-4-methyl]-N-[5-(nitrooxy)-1-oxopentyl]-L-valine, which underwent detritylation to give compound II. All the invention compds. were evaluated for their AT1 inhibitory activity. From the assay, it was determined that compound II exhibited an IC50 value of 19 nM and 86 % inhibition at 100 nM.

IT '167301-42-0D, derivs., nitrate esters

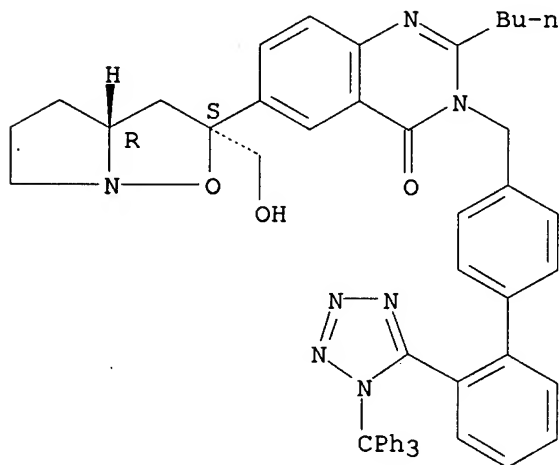
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of benzimidazole-tetrazole-nitric oxide compds. as enhancing angiotensin II antagonist compds. and their use in the treatment of disease)

RN 167301-42-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[(2R,3aS)-hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 3 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1252075 ZCAPLUS

DOCUMENT NUMBER: 146:157754

TITLE: Synthesis and Properties of Size-Expanded DNAs: Toward Designed, Functional Genetic Systems

AUTHOR(S): Krueger, Andrew T.; Lu, Haige; Lee, Alex H. F.; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305, USA

SOURCE: Accounts of Chemical Research (2007), 40(2), 141-150

CODEN: ACHRE4; ISSN: 0001-4842

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We describe the design, synthesis, and properties of DNA-like mols. in which the base pairs are expanded by benzo homologation. The resulting size-expanded genetic helixes are called xDNA ("expanded DNA") and yDNA ("wide DNA"). The large component bases are fluorescent, and they display high stacking affinity. When singly substituted into natural DNA, they are destabilizing because the benzo-expanded base pair size is too large for the natural helix. However, when all base pairs are expanded, xDNA and yDNA form highly stable, sequence-selective double helixes. The size-expanded DNAs are candidates for components of new, functioning genetic systems. In addition, the fluorescence of expanded DNA bases makes them potentially useful in probing nucleic acids.

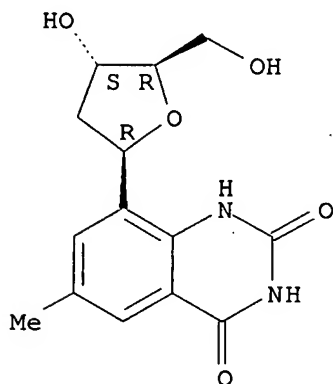
IT 639465-38-6 830343-25-4

RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (synthesis and properties of size-expanded DNAs)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 8-(2-deoxy- β -D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

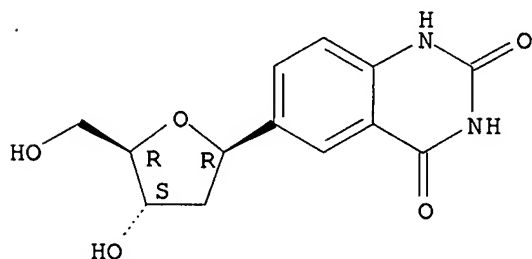
Absolute stereochemistry.



RN 830343-25-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(2-deoxy- β -D-erythro-pentofuranosyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

68

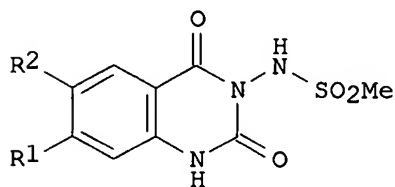
THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1093812 ZCAPLUS
 DOCUMENT NUMBER: 145:419171
 TITLE: Preparation of 1H-quinazoline-2,4-diones as
 AMPA-receptor ligands
 INVENTOR(S): Allgeier, Hans; Auberson, Yves; Carcache, David;
 Floersheim, Philipp; Guibourdenche, Christel; Froestl,
 Wolfgang; Kallen, Joerg; Koller, Manuel; Mattes,
 Henri; Nozulak, Joachim; Orain, David; Renaud, Johanne
 PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H..
 SOURCE: PCT Int. Appl., 157pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006108591	A1	20061019	WO 2006-EP3251	20060410
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: GB 2005-7298 A 20050411
 OTHER SOURCE(S): MARPAT 145:419171
 GI



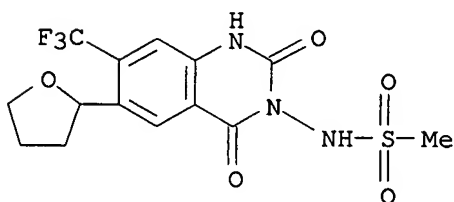
- AB Title compds. represented by the formula I [wherein R1 = CF3, CHF2, CH2F, etc.; R2 = (un)substituted (heterocyclyl)alkyl, heterocyclyl or phenyl; and their salts thereof] were prepared as AMPA-receptor ligands. For example, I (R1 = CF3, R2 = MeCO) was provided in a multi-step synthesis starting from 2-nitro-4-trifluoromethylbenzoic acid. I [R1 = CF3, R2 = EtOCH(Me)] showed AMPA-receptor binding activity with IC50 value of 1 μ M. Thus, title compds. and their pharmaceutical compns. are useful as AMPA-receptor ligands, in particular for the treatment of epilepsy or schizophrenia (no data).
- IT 912573-90-1P, N-[2,4-Dioxo-6-(tetrahydrofuran-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide
 RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of 1H-quinazoline-2,4-diones as AMPA-receptor ligands)

RN 912573-90-1 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(tetrahydro-2-furanyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



IT 912574-83-5P, (S)-N-[2,4-Dioxo-6-(tetrahydrofuran-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide

912574-84-6P, (R)-N-[2,4-Dioxo-6-(tetrahydrofuran-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide

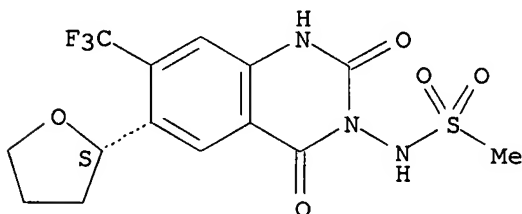
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1H-quinazoline-2,4-diones as AMPA-receptor ligands)

RN 912574-83-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-[(2S)-tetrahydro-2-furanyl]-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

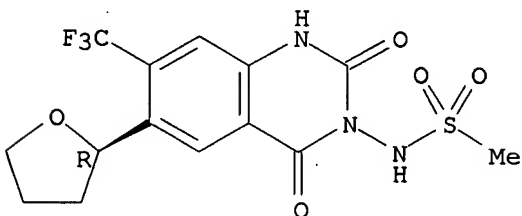
Absolute stereochemistry.



RN 912574-84-6 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-[(2R)-tetrahydro-2-furanyl]-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 912574-05-1P, N-[2,4-Dioxo-6-(tetrahydropyran-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide

912574-33-5P, N-[6-(1-Methyl-1H-pyrrol-2-yl)-2,4-dioxo-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide

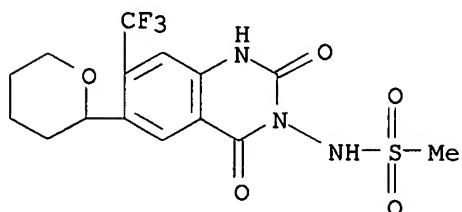
912574-36-8P, N-[2,4-Dioxo-6-(tetrahydrofuran-3-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide
 912574-73-3P, N-[2,4-Dioxo-6-(pyridin-4-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide 912574-74-4P,
 N-[2,4-Dioxo-6-(pyridin-3-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide 912574-75-5P, N-[6-(6-Methoxypyridin-3-yl)-2,4-dioxo-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide 912574-76-6P, N-[2,4-Dioxo-6-(pyridin-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide
 912574-78-8P, N-[2,4-Dioxo-6-(1H-pyrrol-2-yl)-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide 912575-56-5P,
 N-[6-(Oxazol-5-yl)-2,4-dioxo-7-trifluoromethyl-1,4-dihydro-2H-quinazolin-3-yl]methanesulfonamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1H-quinazoline-2,4-diones as AMPA-receptor ligands)

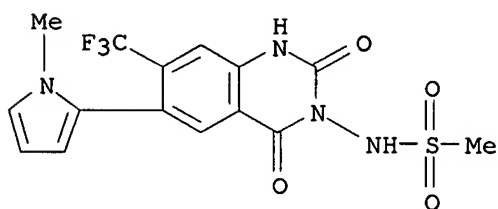
RN 912574-05-1 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(tetrahydro-2H-pyran-2-yl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



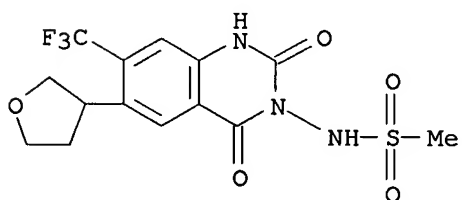
RN 912574-33-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



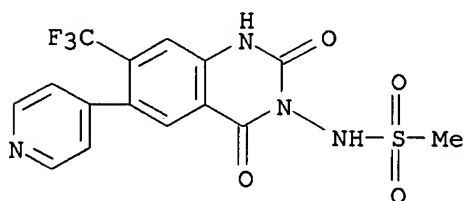
RN 912574-36-8 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(tetrahydro-3-furanyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



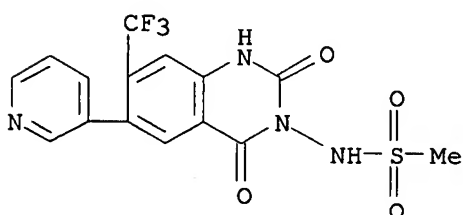
RN 912574-73-3 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(4-pyridinyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



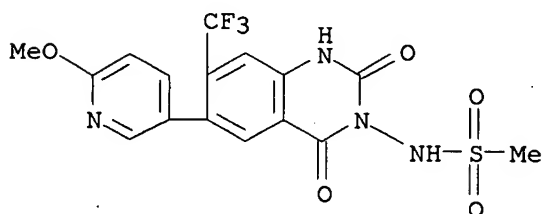
RN 912574-74-4 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(3-pyridinyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



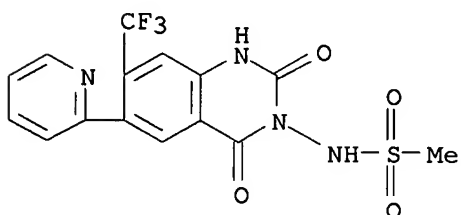
RN 912574-75-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(6-methoxy-3-pyridinyl)-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



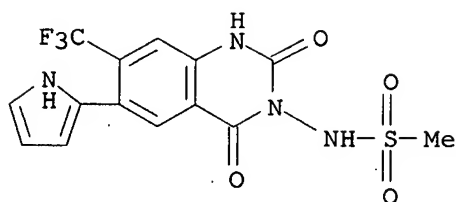
RN 912574-76-6 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(2-pyridinyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



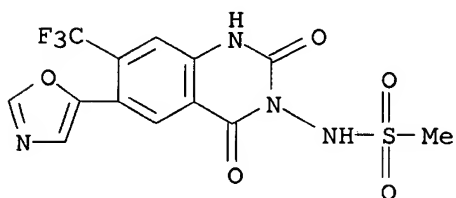
RN 912574-78-8 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(1H-pyrrol-2-yl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 912575-56-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(5-oxazolyl)-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1090222 ZCAPLUS

DOCUMENT NUMBER: 146:57129

TITLE: Toward a Designed, Functioning Genetic System with Expanded-Size Base Pairs: Solution Structure of the Eight-Base xDNA Double Helix

AUTHOR(S): Lynch, Stephen R.; Liu, Haibo; Gao, Jianmin; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA

SOURCE: Journal of the American Chemical Society (2006), 128(45), 14704-14711

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe the NMR-derived solution structure of the double-helical form of a designed eight-base genetic pairing system, termed xDNA. The benzo-homologous xDNA design contains base pairs that are wider than natural DNA pairs by ca. 2.4 Å (the width of a benzene ring). The eight component bases of this xDNA helix are A, C, G, T, xA, xT, xC, and xG. The structure was solved in aqueous buffer using 1D and 2D NMR methods combined with restrained mol. dynamics. The data show that the decamer duplex is right-handed and antiparallel, and hydrogen-bonded in a way analogous to that of Watson-Crick DNA. The sugar-phosphate backbone adopts a regular conformation similar to that of B-form DNA, with small dihedral adjustments due to the larger circumference of the helix. The grooves are much wider and more shallow than those of B-form DNA, and the helix turn is slower, with ca. 12 base pairs per 360° turn. There is an extensive intra- and interstrand base stacking surface area, providing an explanation for the greater stability of xDNA relative to natural DNA. There is also evidence for greater motion in this structure compared to a previous two-base-expanded helix; possible chemical and

structural reasons for this are discussed. The results confirm paired self-assembly of the designed xDNA system. This suggests the possibility that other genetic system structures besides the natural one might be functional in encoding information and transferring it to new complementary strands.

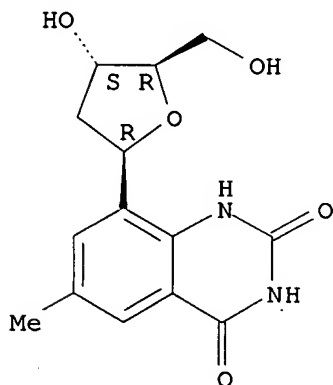
IT 639465-38-6

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(NMR-derived solution structure of eight-base xDNA double helix)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 8-(2-deoxy- β -D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:978593 ZCAPLUS

DOCUMENT NUMBER: 145:348634

TITLE: Organic nitric oxide enhancing salts of angiotensin II antagonists, compositions and methods of use

INVENTOR(S): Garvey, David, S.; Cai, Xiong; Lin, Chia-En; Ranatunge, Ramini, R.; Stevenson, Cheri, A.; Wey, Shiow-Jyi

PATENT ASSIGNEE(S): Nitromed, Inc., USA

SOURCE: PCT Int. Appl., 126pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006099058	A2	20060921	WO 2006-US8441	20060309
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,</p>				

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

US 2005-659401P

P 20050309

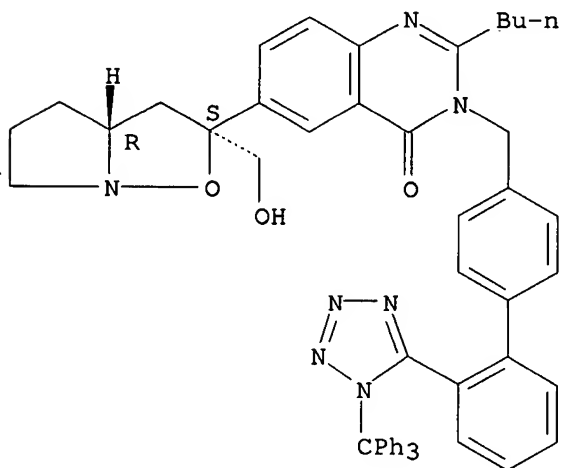
US 2005-750773P

P 20051215

OTHER SOURCE(S): MARPAT 145:348634

- AB The invention describes compns. and kits comprising at least one organic nitric oxide enhancing salt of an angiotensin II antagonist, and, optionally, at least one nitric oxide enhancing compound and/or at least one therapeutic agent. The invention also provides methods for (a) treating cardiovascular diseases; (b) treating renovascular diseases; (c) treating diabetes; (d) treating diseases resulting from oxidative stress; (e) treating endothelial dysfunctions; (f) treating diseases caused by endothelial dysfunctions; (g) treating cirrhosis; (h) treating pre-eclampsia; (j) treating osteoporosis; (k) treating nephropathy; (l) treating peripheral vascular diseases; (m) treating portal hypertension; (n) treating ophthalmic disorders; (o) treating metabolic syndrome; and (p) treating hyperlipidemia. The organic nitric oxide enhancing compds. that form salts with the angiotensin II antagonists are organic nitrates, organic nitrites, nitrosothiols, thionitrites, thionitrates, NONOates, heterocyclic nitric oxide donors and/or nitroxides. The heterocyclic nitric oxide donors are furoxans, sydnonimines, oxatriazole-5-ones and/or oxatriazole-5-imines.
- IT 167301-42-0D, organic nitric oxide enhancing salts
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (organic nitric oxide enhancing salts of angiotensin II antagonists for treatment of diseases and combination with other agents)
- RN 167301-42-0 ZCAPLUS
- CN 4(3H)-Quinazolinone, 2-butyl-6-[(2R,3aS)-hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 7 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:937683 ZCAPLUS

DOCUMENT NUMBER: 145:471484

TITLE: Structural Investigation of the 7-Chloro-3-hydroxy-1H-quinazoline-2,4-dione Scaffold to Obtain AMPA and Kainate Receptor Selective Antagonists. Synthesis, Pharmacological, and Molecular Modeling Studies

AUTHOR(S): Colotta, Vittoria; Catarzi, Daniela; Varano, Flavia; Lenzi, Ombretta; Filacchioni, Guido; Costagli, Chiara; Galli, Alessandro; Ghelardini, Carla; Galeotti, Nicoletta; Gratteri, Paola; Sgrignani, Jacopo; Deflorian, Francesca; Moro, Stefano

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Laboratorio di Progettazione, Sintesi e Studio di Eterocicli Biologicamente Attivi, Polo Scientifico, Universita degli Studi di Firenze, Sesto Fiorentino (FI), 50019, Italy

SOURCE: Journal of Medicinal Chemistry (2006), 49(20), 6015-6026
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

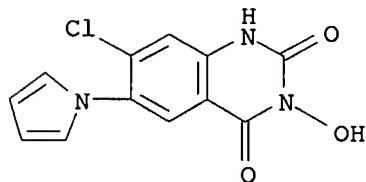
OTHER SOURCE(S): CASREACT 145:471484

AB In this paper, the study of new 7-chloro-3-hydroxy-1H-quinazoline-2,4-dione derivs., designed as AMPA and kainate (KA) receptor antagonists, is reported. Some derivs. bear different carboxy-containing alkyl chains on the 3-hydroxy group, while various heterocyclic rings or amide moieties are present at the 6-position of other compds. Binding data at Gly/NMDA, AMPA, and high-affinity KA receptors showed that the presence of the free 3-hydroxy group is of paramount importance for a good affinity at all three investigated receptors, while introduction of some 6-heterocyclic moieties yielded AMPA-selective antagonists. The most significant result was the finding of the 6-(2-carboxybenzoylamino)-3-hydroxy-1H-quinazoline-2,4-dione, which possesses good affinity for high-affinity and low-affinity KA receptors ($K_i = 0.62 \mu\text{M}$ and $1.6 \mu\text{M}$, resp.), as well as good selectivity. To rationalize the trend of affinities of the reported derivs., an intensive mol. modeling study was carried out by docking compds. to models of the Gly/NMDA, AMPA, and KA receptors.

IT 913973-76-9P 913973-80-5P 913973-83-8P
913973-86-1P 913973-89-4P 913973-93-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 7-chloro-3-hydroxy-1H-quinazoline-2,4-dione derivs. as AMPA and kainate receptor antagonists)

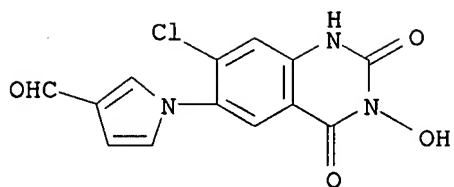
RN 913973-76-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 7-chloro-3-hydroxy-6-(1H-pyrrol-1-yl)- (9CI)
(CA INDEX NAME)



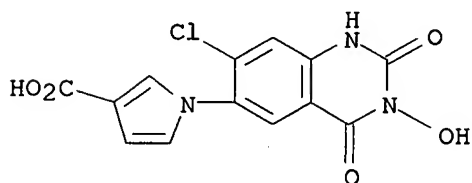
RN 913973-80-5 ZCAPLUS

CN 1H-Pyrrole-3-carboxaldehyde, 1-(7-chloro-1,2,3,4-tetrahydro-3-hydroxy-2,4-dioxo-6-quinazolinyl)- (9CI) (CA INDEX NAME)



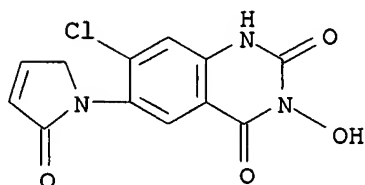
RN 913973-83-8 ZCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(7-chloro-1,2,3,4-tetrahydro-3-hydroxy-2,4-dioxo-6-quinazolinyl)- (9CI) (CA INDEX NAME)



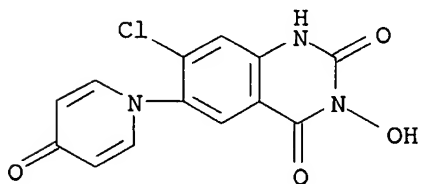
RN 913973-86-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-chloro-6-(2,5-dihydro-2-oxo-1H-pyrrol-1-yl)-3-hydroxy- (9CI) (CA INDEX NAME)



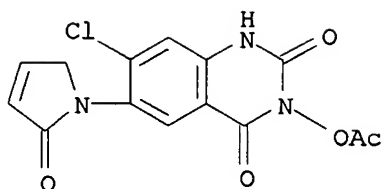
RN 913973-89-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-chloro-3-hydroxy-6-(4-oxo-1(4H)-pyridinyl)- (9CI) (CA INDEX NAME)



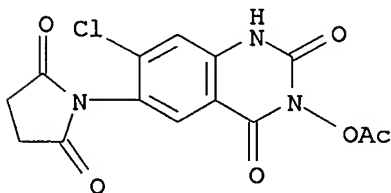
RN 913973-93-0 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-chloro-6-(2,5-dioxo-1-pyrrolidinyl)-3-hydroxy- (9CI) (CA INDEX NAME)



RN 913974-19-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 3-(acetyloxy)-7-chloro-6-(2,5-dioxo-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:917623 ZCAPLUS

DOCUMENT NUMBER: 145:306813

TITLE: Cardiovascular compounds comprising nitric oxide enhancing groups, compositions, and methods of use
Garvey, David S.

INVENTOR(S):
PATENT ASSIGNEE(S): Nitromed, Inc., USA

SOURCE: PCT Int. Appl., 140pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006093864	A1	20060908	WO 2006-US6843	20060228
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: US 2005-656544P P 20050228

OTHER SOURCE(S): MARPAT 145:306813

AB The invention describes compns. and kits comprising at least one cardiovascular compound comprising at least one nitric oxide enhancing

group, or pharmaceutically acceptable salts thereof, and, optionally, at least one nitric oxide enhancing compound and/or at least one therapeutic agent. The invention also provides methods for (a) treating cardiovascular diseases; (b) treating renovascular diseases; (c) treating diabetes; (d) treating diseases resulting from oxidative stress; (e) treating endothelial dysfunctions; (f) treating diseases caused by endothelial dysfunctions; (g) treating cirrhosis; (h) treating pre-eclampsia; (i) treating osteoporosis; (j) treating nephropathy; (k) treating peripheral vascular diseases; (l) treating portal hypertension; (m) treating ophthalmic disorders; (n) treating metabolic syndrome; and (o) treating hyperlipidemia. The cardiovascular compds. are angiotensin II antagonists, aldosterone antagonists, endothelin antagonists, hydralazine compds., neutral endopeptidase inhibitors and renin inhibitors. The nitric oxide enhancing groups are nitroxides and/or heterocyclic nitric oxide donors.

IT 167301-42-0D, NO-enhancing derivs.

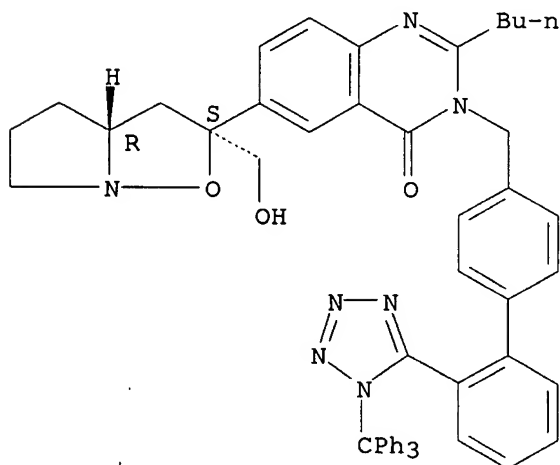
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cardiovascular compds. comprising nitric oxide enhancing groups, compns., and methods of use)

RN 167301-42-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[(2R,3aS)-hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:629586 ZCAPLUS

DOCUMENT NUMBER: 145:293284

TITLE: Exploring the Limits of DNA Size: Naphtho-Homologated DNA Bases and Pairs

AUTHOR(S): Lee, Alex H. F.; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305, USA

SOURCE: Journal of the American Chemical Society (2006), 128(28), 9219-9230

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:293284

AB A new design for DNA bases and base pairs is described in which the pyrimidine bases are widened by naphtho-homologation. Two naphtho-homologated deoxyribosides, dyyT (1) and dyyC (2), were synthesized and could be incorporated into oligonucleotides as suitably protected phosphoramidite derivs. The deoxyribosides were found to be fluorescent, with emission maxima at 446 and 433 nm, resp. Studies with single substitutions of 1 and 2 in the natural DNA context revealed exceptionally strong base stacking propensity for both. Sequences containing multiple substitutions of 1 and 2 paired opposite adenine and guanine were subsequently mixed and studied by several anal. methods. Data from UV mixing expts., FRET measurements, fluorescence quenching expts., and hybridizations on beads suggest that complementary "double-wide DNA" (yyDNA) strands may self-assemble into helical complexes with 1:1 stoichiometry. Data from thermal denaturation plots and CD spectra were less conclusive. Control expts. in one sequence context gave evidence that yyDNA helices, if formed, are preferentially antiparallel and are sequence. Hypothesized base pairing schemes are analogous to Watson-Crick pairing, but with glycosidic C1'-C1' distances widened by over 45%, to ca. 15.2 Å. The possible self-assembly of the double-wide DNA helix establishes a new limit for the size of information-encoding, DNA-like mols., and the fluorescence of yyDNA bases suggests uses as reporters in monomeric and oligomeric forms.

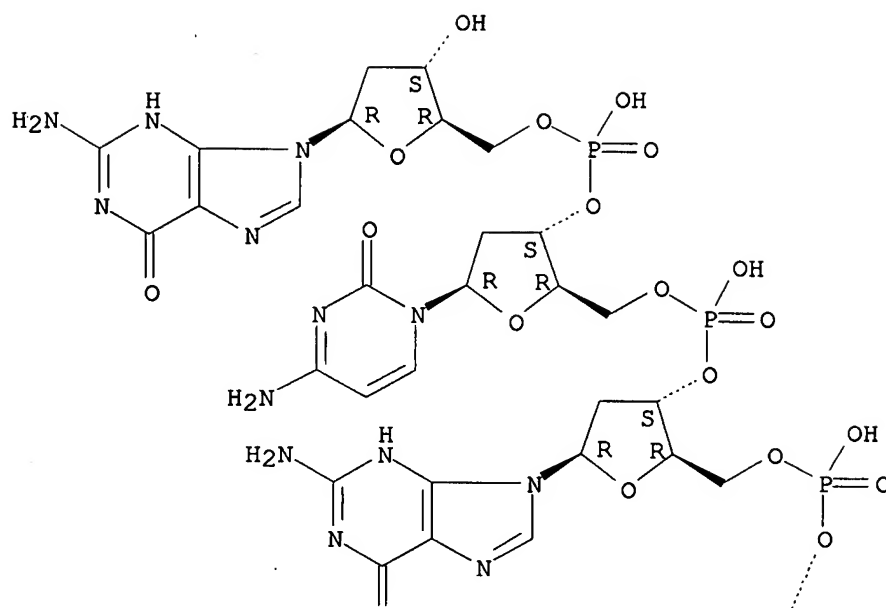
IT 830343-53-8P 906546-13-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and exploring limits of DNA size of naphtho-homologated DNA bases and pairs)

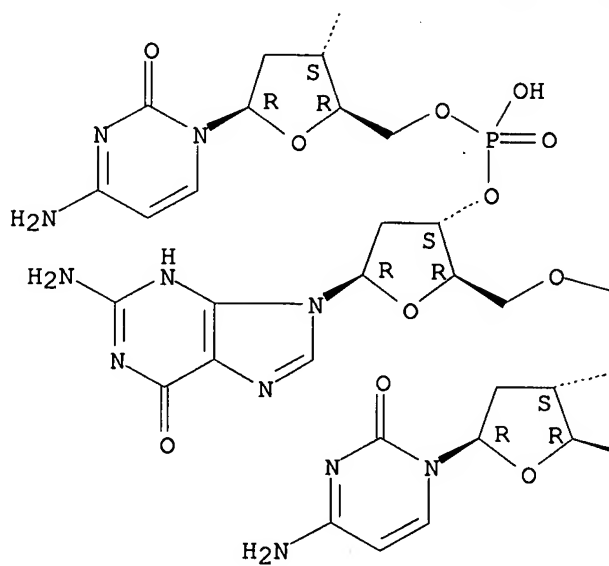
RN 830343-53-8 ZCAPLUS

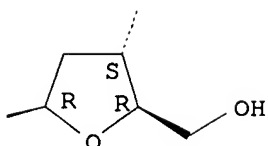
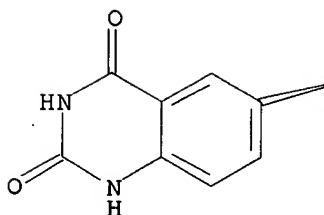
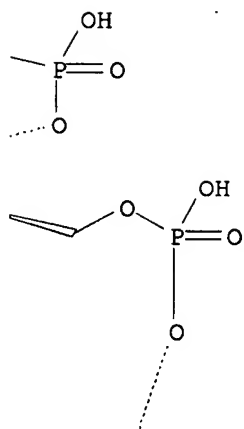
CN Guanosine, 1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



O

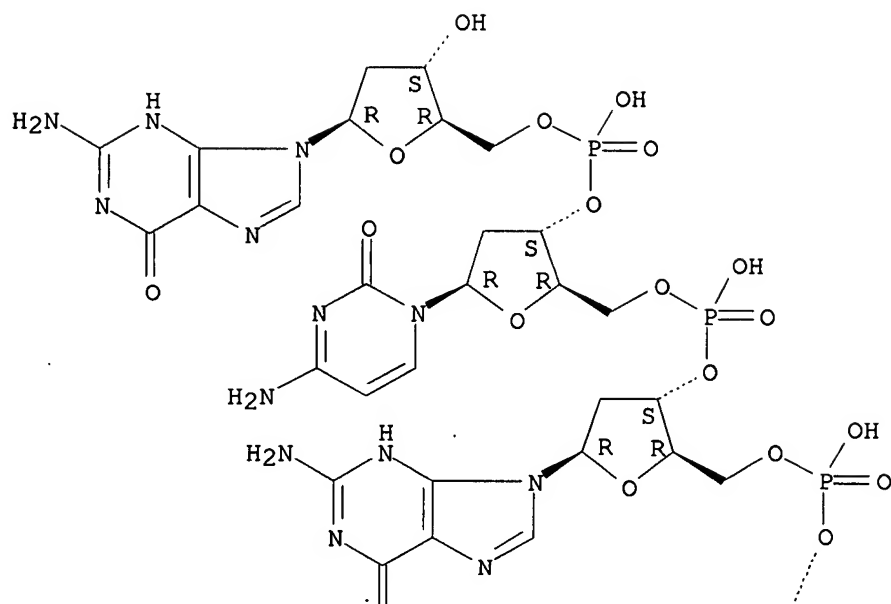




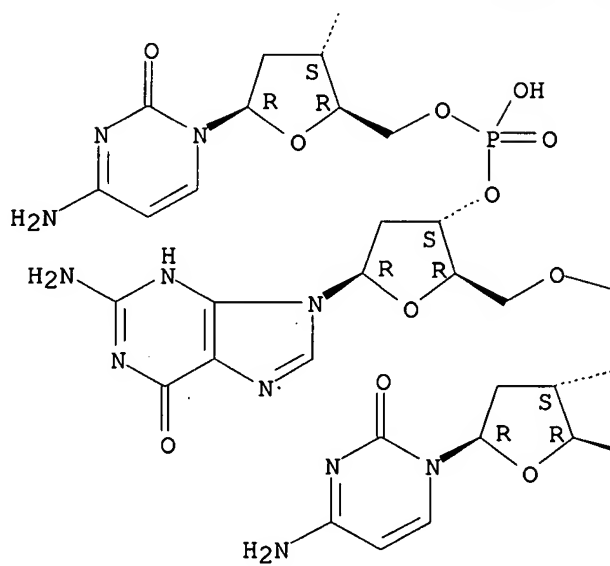
RN 906546-13-2 ZCAPLUS

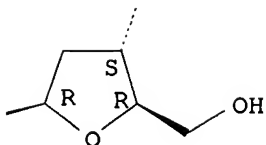
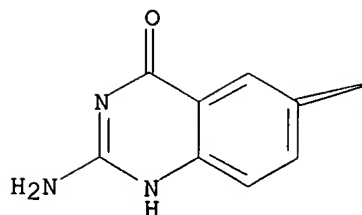
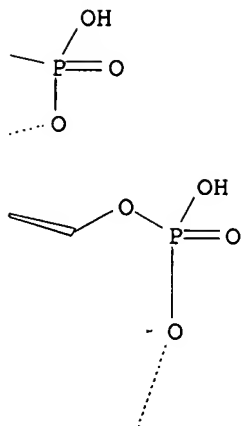
CN Guanosine, 1'-(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenyl-yl-(3'→5')-2'-deoxycytidyl-yl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidyl-yl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidyl-yl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



O





REFERENCE COUNT:

68

THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:465188 ZCAPLUS

DOCUMENT NUMBER: 144:488667

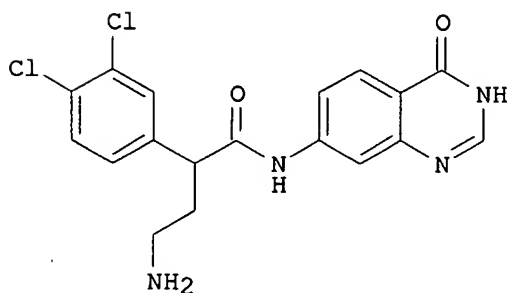
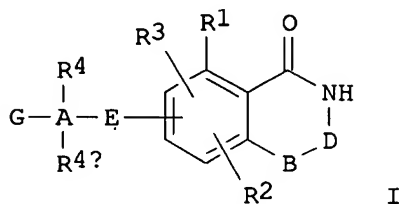
TITLE: Pharmaceutical compounds such as quinazolinones and
their preparation, and use for treatment of protein
kinase A and/or B mediated diseases

INVENTOR(S): Berdini, Valerio; Boyle, Robert George; Saxty, Gordon;

Verdonk, Marinus Leendert; Woodhead, Steven John;
Wyatt, Paul Graham; Sore, Hannah Fiona; Walker, David
Winter; Caldwell, John; Collins, Ian
PATENT ASSIGNEE(S): Astex Therapeutics Limited, UK; The Institute of
Cancer ResearchRoyal Cancer Hospital; Cancer Research
Technology Limited
SOURCE: PCT Int. Appl., 178 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006051290	A2	20060518	WO 2005-GB4323	20051109
WO 2006051290	A3	20060914		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: GB 2004-24742 A 20041109
US 2004-626403P P 20041109
OTHER SOURCE(S): MARPAT 144:488667
GI



AB The invention is related to quinazolinones I [B-D = N:CH and derivs., NHCO and derivs.; G = OH, NH2 ad derivs.; E = CONH and derivs., O, S, NH, etc.,

with proviso; A = a bond and R4 and R4a are absent; or A = saturated hydrocarbon linker containing 1-7 C's, wherein 1 of the C atoms may optionally be replaced by an O or N atom; R1-R3 = independently H, halo, (un)substituted hydrocarbyl; R4 = H, alkyl; R4a = H, alkyl, monocyclic or bicyclic carbocyclyl or heterocyclyl containing up to 3 heteroatoms; or R4 and R4a together with the intervening atom(s) of A form a saturated monocyclic heterocyclic group] or salts, solvates, tautomers or N-oxides thereof, that inhibit or modulate the activity of protein kinase A (PKA) and protein kinase B (PKB), and their use in the treatment or prophylaxis of disease states or conditions mediated by PKA and PKB, such as proliferative diseases. The invention is also related to the preparation of quinazolinones I. Thus, acylation of 4-[(tert-butoxycarbonyl)amino]-2-(3,4-dichlorophenyl)butyric acid with 7-amino-3H-quinazolin-4-one and Boc-deprotection gave quinazolinone II. Selected I inhibited protein kinase A and/or B with IC50 values of less than 50 μ M.

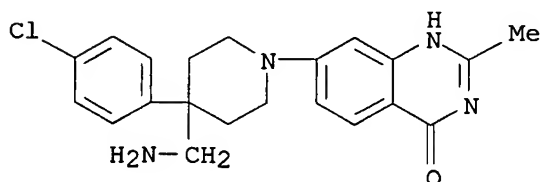
IT 887129-14-8P, 7-[4-Aminomethyl-4-(4-chlorophenyl)piperidin-1-yl]-2-methyl-3H-quinazolin-4-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinazolinones as protein kinase A and/or B inhibitors for treating proliferative diseases)

RN 887129-14-8 ZCAPLUS

CN 4(1H)-Quinazolinone, 7-[4-(aminomethyl)-4-(4-chlorophenyl)-1-piperidinyl]-2-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:153587 ZCAPLUS

DOCUMENT NUMBER: 144:331393

TITLE: Synthesis of 5-heterocyclic substituted quinazolin-4-ones via 2-aminobenzonitrile derivatives

AUTHOR(S): Fray, M. Jonathan; Allen, Paul; Bradley, Paul R.; Challenger, Clare E.; Closier, Michael; Evans, Tim J.; Lewis, Mark L.; Mathias, John P.; Nichols, Carly L.; Po-Ba, Yvonne M.; Snow, Hayley; Stefaniak, Mark H.; Vuong, Hannah V.

CORPORATE SOURCE: Department of Discovery Chemistry, Pfizer Global Research and Development, Sandwich, Kent, CT13 9NJ, UK

SOURCE: Heterocycles (2006), 67(2), 489-494

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:331393

AB Two routes to prepare a series of six 5-heterocyclic substituted 2-chloro-7-methoxyquinazolin-4-ones are described, where the heterocycle is a substituted or unsubstituted 1-pyrazolyl, 5-pyrazolyl, or 2-thiazolyl group. Both routes proceeded via key 2-aminobenzonitrile intermediates.

IT 880885-48-3P

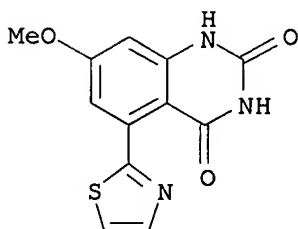
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of heterocyclic substituted quinazolinones via aminobenzonitriles)

RN 880885-48-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 7-methoxy-5-(2-thiazolyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:104528 ZCAPLUS

DOCUMENT NUMBER: 144:192275

TITLE: Preparation of quinazolinone derivatives useful for the regulation of glucose homeostasis and food intake

INVENTOR(S): Rudolph, Joachim; O'Connor, Stephen; Coish, Philip; Wickens, Philip; Bondar, Georgiy; Chuang, Chih-Yuan; Ramsden, Philip; Lowe, Derek; Bierer, Donald; Chen, Libing; Fu, Wenlang; Khire, Uday; Liu, Xiao-Gao; McClure, Andrea; Wang, Lei; Yi, Lin; Esler, William

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 559 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006012577	A2	20060202	WO 2005-US26192	20050722
WO 2006012577	A3	20060928		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: US 2004-590804P P 20040722

OTHER SOURCE(S): MARPAT 144:192275

GI

neuropathic pain, affective and attention disorders, schizophrenia, tinnitus, myopia and other ocular disorders, multiple sclerosis, dementia. The invention provides a combination which comprises at least one compound I ("AMPA receptor antagonist") and at least one compound selected from the group consisting of lithium, valproic acid sodium salt, conventional antipsychotics, atypical antipsychotics, lamotrigine, Me phenidate, antidepressants and antiepileptics is greater than the additive effect of the combined drugs. Thus, quinazoline II was prepared and tested as an antagonist at the rGluR3 AMPA receptor with an IC₅₀ of 2.3 μ M.

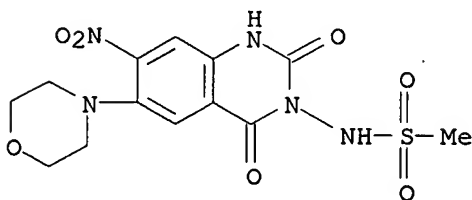
IT 875154-00-0P 875154-06-6P 875154-07-7P
875154-08-8P 875154-34-0P 875154-37-3P
875154-52-2P 875154-53-3P 875154-54-4P
875154-65-7P 875154-71-5P 875154-72-6P
875154-73-7P 875154-74-8P 875154-75-9P
875154-76-0P 875154-83-9P 875154-94-2P
875154-95-3P 875154-99-7P 875155-01-4P
875155-02-5P 875155-03-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazoline derivs. as AMPA receptor antagonist and for the treatment or delay of progression of epilepsy or schizophrenia)

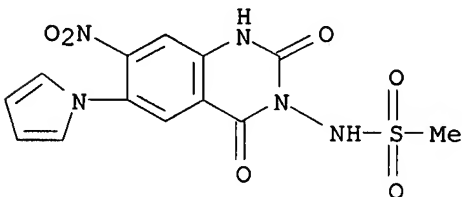
RN 875154-00-0 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(4-morpholinyl)-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



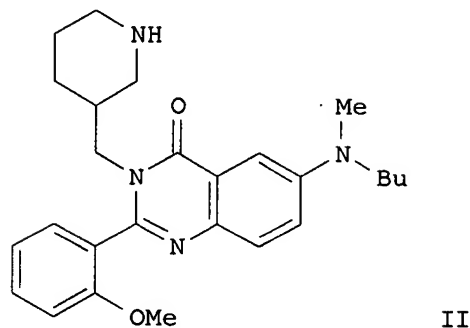
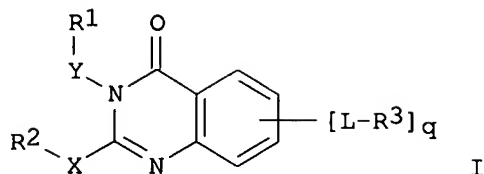
RN 875154-06-6 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-7-nitro-2,4-dioxo-6-(1H-pyrrol-1-yl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 875154-07-7 ZCAPLUS

CN Methanesulfonamide, N-[6-(3-formyl-1H-pyrrol-1-yl)-1,4-dihydro-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



AB The invention is related to substituted quinazolinone derivs. I [R1 = (un)substituted pyrrolidin-3-yl, piperidin-3-yl, morpholin-4-yl, etc.; R2 = H, (un)substituted cyclo/alkyl, pyridinyl, Ph, etc.; R3 = H, halo, haloalkyl, (un)substituted Ph, alkyl, etc.; L = a bond, O, CO, S, SO2, NHSO2, NH and derivs., etc.; X = (CH2)m; m = 0-2; Y = (CH2)n; n = 1-2; p = 0-2; with provisos], and their pharmaceutically acceptable salts, and their compns., and methods for treating diabetes, obesity and related disorders, and regulation of glucose homeostasis and food intake (e.g., stimulation and suppression) (no data). The invention is also related to the preparation of quinazolinones I. Five biol. tests are given (no data). Thus, II•TFA was prepared by amination of 5-fluoro-2-nitrobenzoic acid with N-methylbutylamine, reduction of the nitro compound, cyclocondensation

with

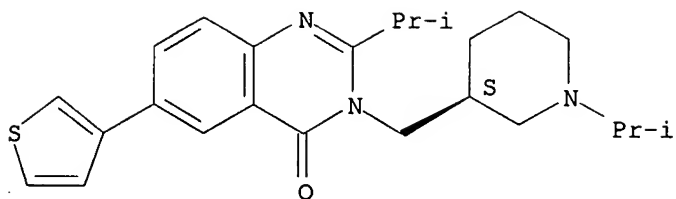
o-anisoyl chloride, reaction with tert-Bu 3-(aminomethyl)piperidine-1-carboxylate (intermediate not isolated), and Boc-deprotection in the presence of TFA.

IT 875259-29-3P, (S)-6-(1,3-Benzodioxol-5-yl)-2-isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]quinazolin-4(3H)-one 875265-48-8P, (S)-2-Isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]-6-(2-thienyl)quinazolin-4(3H)-one 875265-51-3P, (S)-2-Isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]-6-(6-methoxypyridin-3-yl)quinazolin-4(3H)-one 875265-56-8P, 6-(3-Furyl)-2-isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]quinazolin-4(3H)-one 875265-63-7P, (S)-2-Isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]-6-(3-thienyl)quinazolin-4(3H)-one 875265-73-9P, (S)-6-(5-Acetyl-2-thienyl)-2-isopropyl-3-[(1-isopropylpiperidin-3-yl)methyl]quinazolin-4(3H)-one 875267-58-6P, (S)-6-(1,3-Benzodioxol-5-yl)-3-[(1-isopropylpiperidin-3-yl)methyl]-2-methylquinazolin-4(3H)-one
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinazolinones useful for regulation of glucose homeostasis and food intake)

RN 875259-29-3 ZCAPLUS

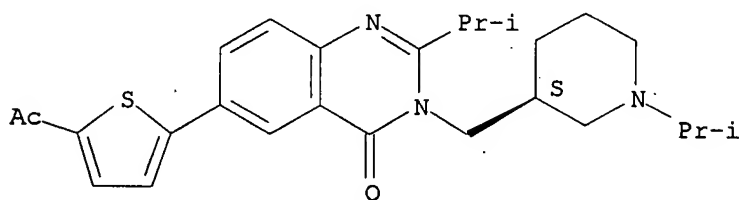
CN 4(3H)-Quinazolinone, 6-(1,3-benzodioxol-5-yl)-2-(1-methylethyl)-3-[(1-methylethyl)-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



RN 875265-73-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(5-acetyl-2-thienyl)-2-(1-methylethyl)-3-[[(3S)-1-(1-methylethyl)-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

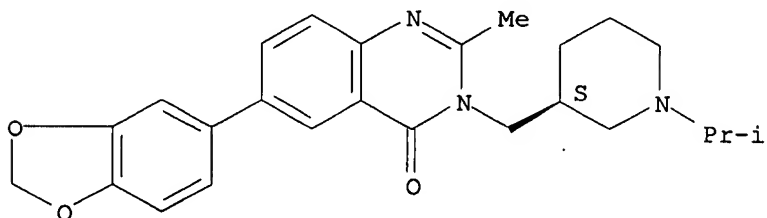
Absolute stereochemistry.



RN 875267-58-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(1,3-benzodioxol-5-yl)-2-methyl-3-[[(3S)-1-(1-methylethyl)-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 13 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:101023 ZCAPLUS

DOCUMENT NUMBER: 144:192265

TITLE: Preparation of quinazoline derivatives as AMPA receptor antagonist and for the treatment or delay of progression of epilepsy or schizophrenia

INVENTOR(S): Allgeier, Hans; Froestl, Wolfgang; Koller, Manuel; Mattes, Henri; Nozulak, Joachim; Ofner, Silvio; Orain, David; Rasetti, Vittorio; Renaud, Johanne; Soldermann, Nicolas; Floersheim, Philipp

PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH

SOURCE: PCT Int. Appl., 122 pp.

CODEN: PIXXD2

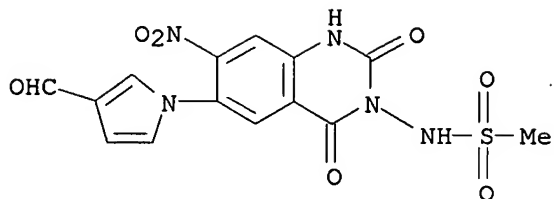
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

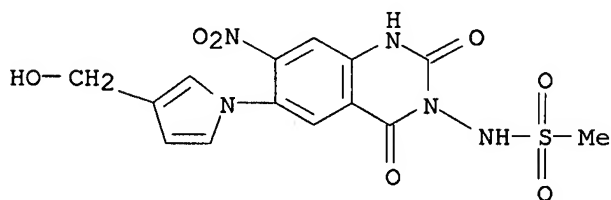
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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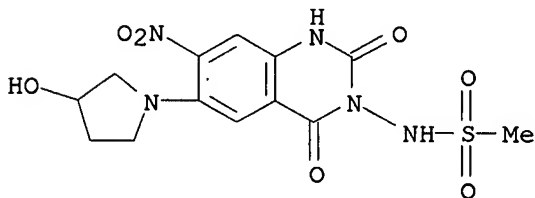
RN 875154-08-8 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-[3-(hydroxymethyl)-1H-pyrrol-1-yl]-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



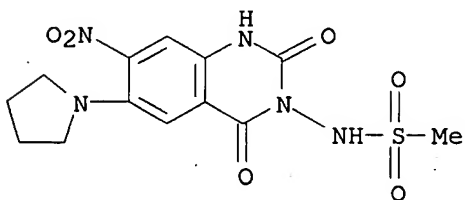
RN 875154-34-0 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(3-hydroxy-1-pyrrolidinyl)-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 875154-37-3 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-7-nitro-2,4-dioxo-6-(1-pyrrolidinyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

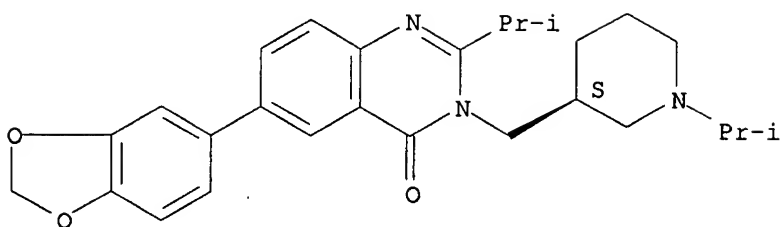


RN 875154-52-2 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-[(3S)-3-hydroxy-1-pyrrolidinyl]-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

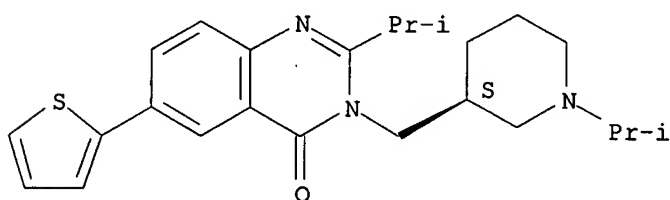
Absolute stereochemistry.



RN 875265-48-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-(1-methylethyl)-3-[[1-(1-methylethyl)-3-piperidinyl]methyl]-6-(2-thienyl)- (9CI) (CA INDEX NAME)

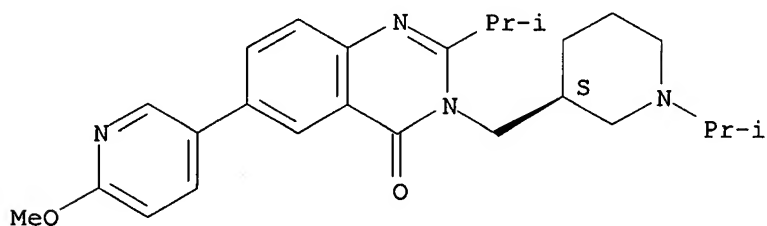
Absolute stereochemistry.



RN 875265-51-3 ZCAPLUS

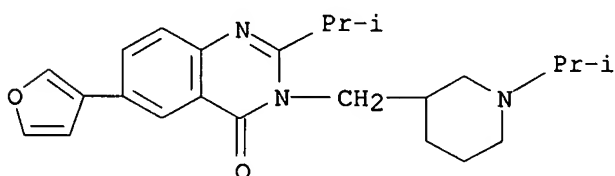
CN 4(3H)-Quinazolinone, 6-(6-methoxy-3-pyridinyl)-2-(1-methylethyl)-3-[[1-(1-methylethyl)-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 875265-56-8 ZCAPLUS

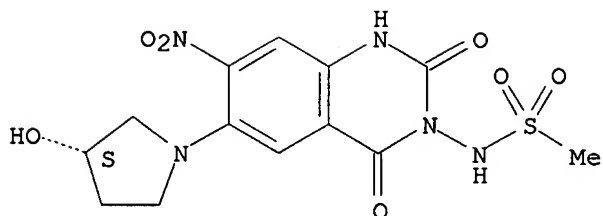
CN 4(3H)-Quinazolinone, 6-(3-furanyl)-2-(1-methylethyl)-3-[[1-(1-methylethyl)-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



RN 875265-63-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-(1-methylethyl)-3-[[1-(1-methylethyl)-3-piperidinyl]methyl]-6-(3-thienyl)- (9CI) (CA INDEX NAME)

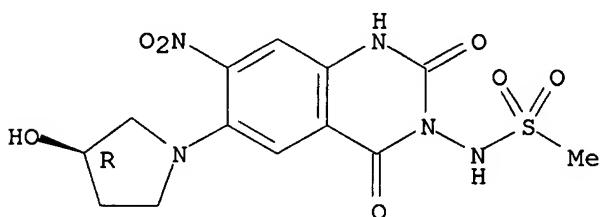
Absolute stereochemistry.



RN 875154-53-3 ZCAPLUS

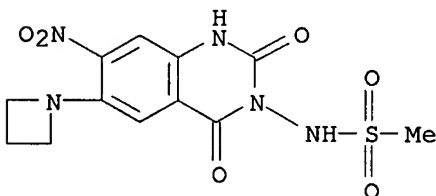
CN Methanesulfonamide, N-[1,4-dihydro-6-[(3R)-3-hydroxy-1-pyrrolidinyl]-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



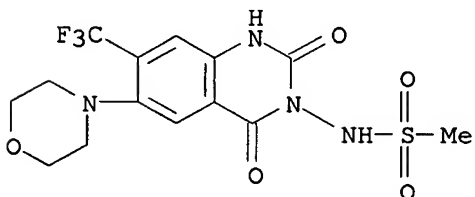
RN 875154-54-4 ZCAPLUS

CN Methanesulfonamide, N-[6-(1-azetidiny)-1,4-dihydro-7-nitro-2,4-dioxo-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



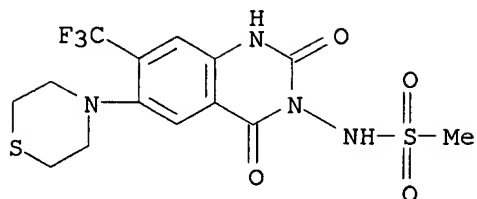
RN 875154-65-7 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(4-morpholinyl)-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



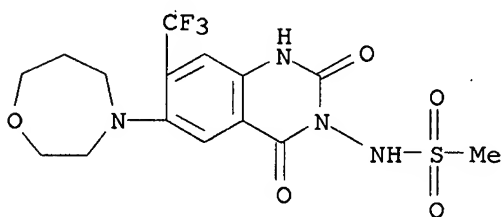
RN 875154-71-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(4-thiomorpholinyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



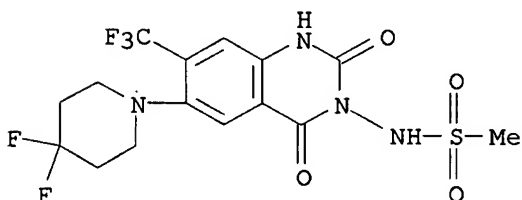
RN 875154-72-6 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(tetrahydro-1,4-oxazepin-4(5H)-yl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



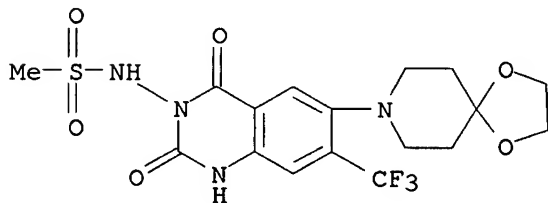
RN 875154-73-7 ZCAPLUS

CN Methanesulfonamide, N-[6-(4,4-difluoro-1-piperidiny)-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 875154-74-8 ZCAPLUS

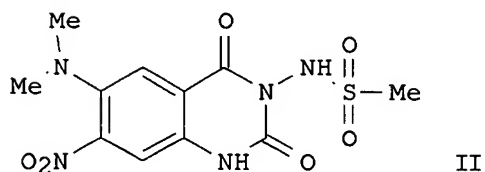
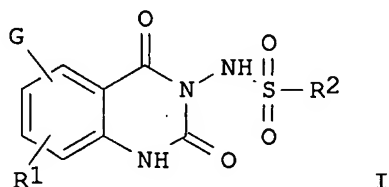
CN Methanesulfonamide, N-[6-(1,4-dioxo-8-azaspiro[4.5]dec-8-yl)-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



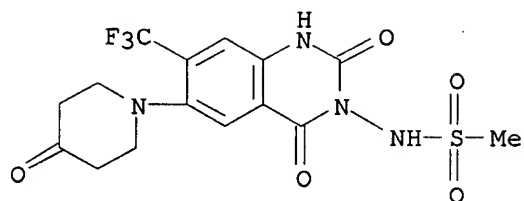
RN 875154-75-9 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(4-oxo-1-piperidiny)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)

WO 2006010591	A2	20060202	WO 2005-EP8113	20050726
WO 2006010591	A3	20061012		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005266490	A1	20060202	AU 2005-266490	20050726
CA 2571223	A1	20060202	CA 2005-2571223	20050726
EP 1773788	A2	20070418	EP 2005-768294	20050726
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
PRIORITY APPLN. INFO.:			GB 2004-16730	A 20040727
			WO 2005-EP8113	W 20050726
OTHER SOURCE(S):		MARPAT 144:192265		
GI				

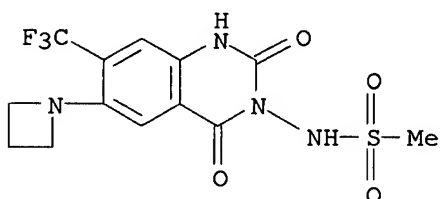


AB 1H-quinazoline-2,4-dione derivs. I, wherein G is NR₃R₄ or OR₅, wherein R₃-R₅ are independently hydrogen, aryl, aralkyl, acyl, alkyl optionally substituted by aryl, heterocyclyl, aryloxy, aralkyloxy or alkoxy-carbonylamino, or R₃ and R₄ together with the adjacent nitrogen atom form heteroaryl or heterocyclyl containing at least one nitrogen ring atom and attached via this nitrogen ring atom, wherein heteroaryl and heterocyclyl are optionally substituted by aryl, aralkyl, aryloxyalkyl, aminocarbonylalkyl, mono- or dialkyl aminocarbonylalkyl or morpholinocarbonylalkyl, R₁ is nitro or trifluoromethyl, and R₂ is alkyl, aryl or aralkyl, and their salts, were prepared as as AMPA receptor antagonist and for the treatment or delay of progression of epilepsy or schizophrenia. Title compds. were prepared and used for the prevention, treatment or delay of progression of epilepsy or schizophrenia,



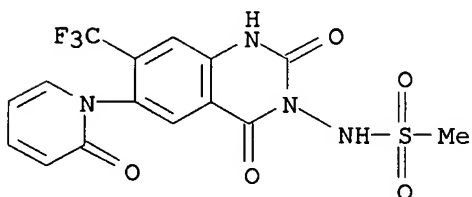
RN 875154-76-0 ZCAPLUS

CN Methanesulfonamide, N-[6-(1-azetidinyl)-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



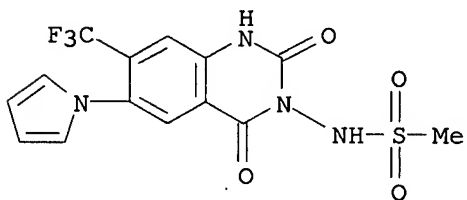
RN 875154-83-9 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(2-oxo-1(2H)-pyridinyl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



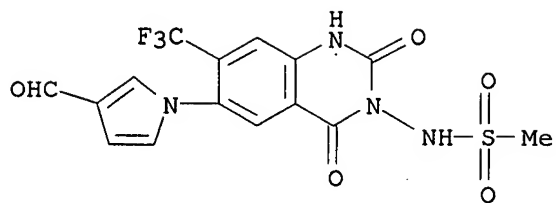
RN 875154-94-2 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-2,4-dioxo-6-(1H-pyrrol-1-yl)-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



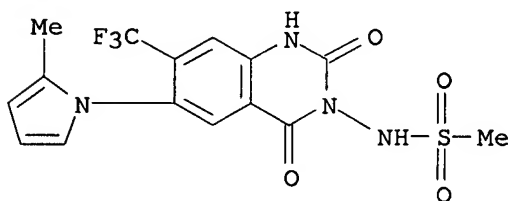
RN 875154-95-3 ZCAPLUS

CN Methanesulfonamide, N-[6-(3-formyl-1H-pyrrol-1-yl)-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



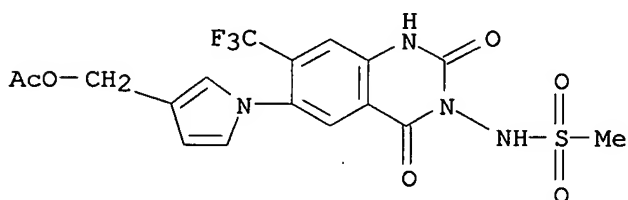
RN 875154-99-7 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-(2-methyl-1H-pyrrol-1-yl)-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



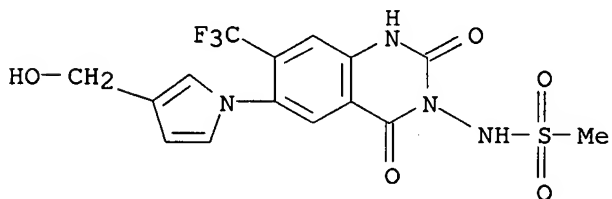
RN 875155-01-4 ZCAPLUS

CN Methanesulfonamide, N-[6-[3-[(acetyloxy)methyl]-1H-pyrrol-1-yl]-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



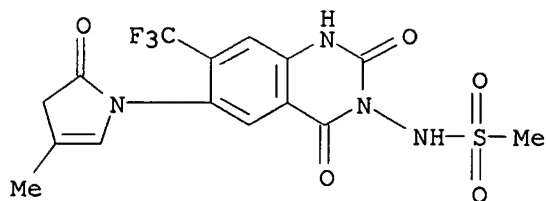
RN 875155-02-5 ZCAPLUS

CN Methanesulfonamide, N-[1,4-dihydro-6-[3-(hydroxymethyl)-1H-pyrrol-1-yl]-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 875155-03-6 ZCAPLUS

CN Methanesulfonamide, N-[6-(2,3-dihydro-4-methyl-2-oxo-1H-pyrrol-1-yl)-1,4-dihydro-2,4-dioxo-7-(trifluoromethyl)-3(2H)-quinazolinyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:32063 ZCAPLUS
 DOCUMENT NUMBER: 144:121798
 TITLE: Tissue factor production inhibitors containing LXR ligands
 INVENTOR(S): Terasaka, Naoki; Hiroshima, Ayano
 PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan
 SOURCE: PCT Int. Appl., 261 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006004030	A1	20060112	WO 2005-JP12185	20050701
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM CA 2572872 A1 20060112 CA 2005-2572872 20050701 EP 1764075 A1 20070321 EP 2005-755860 20050701 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR PRIORITY APPLN. INFO.: JP 2004-196468 A 20040702 WO 2005-JP12185 W 20050701				

OTHER SOURCE(S): MARPAT 144:121798

AB Disclosed is a pharmaceutical having the potency of inhibiting the production of tissue factors, which pharmaceutical comprises an LXR ligand as an active ingredient. There is provided a pharmaceutical for the treatment and/or prevention of vascular re-stenosis encountered after angioplasty, endarterectomy, percutaneous coronary angioplasty (PTCA) or stent placement, or for the treatment and/or prevention of blood coagulation disorder, diseases induced by platelet aggregation including stable or unstable angina, disorders of cardiovascular and cerebrovascular systems including thromboembolism induced by diabetes, re-thrombosis encountered after thrombolysis, brain ischemia seizure, infarction, apoplexy, dementia resulting from ischemia, peripheral arterial disease, thromboembolism encountered during the use of aortocoronary bypass, glomerulosclerosis, kidney embolism, tumor or cancer metastasis, which pharmaceutical comprises an LXR ligand as an active ingredient. For example, a compound

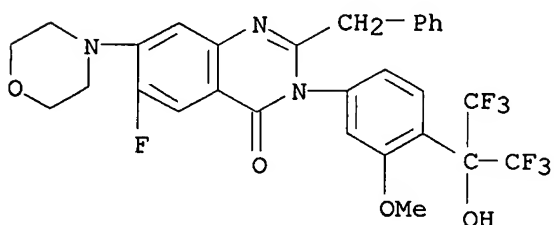
6-chloro-7-methoxy-3-[2-methyl-5-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(3-thienylmethyl)-4(3H)-quinazoline (I) was prepared, and examined for its tissue factor production inhibitory effect. Also, a capsule containing I 100, lactose 150, cellulose 50, and magnesium stearate 6 mg was formulated.

IT 848091-40-7 848092-29-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tissue factor production inhibitors containing LXR ligands)

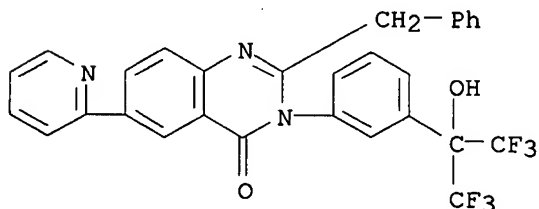
RN 848091-40-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-3-[3-methoxy-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-7-(4-morpholinyl)-2-(phenylmethyl)- (9CI)
(CA INDEX NAME)



RN 848092-29-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(2-pyridinyl)-3-[3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4. THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1350718 ZCAPLUS

DOCUMENT NUMBER: 144:88308

TITLE: Preparation of substituted quinazolones as B-Raf kinase inhibitors for the treatment of cancer

INVENTOR(S): Aquila, Brian; Dakin, Les; Ezhuthachan, Jayachandran; Lee, John; Lyne, Paul; Pontz, Timothy

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005123696	A1	20051229	WO 2005-GB2327	20050614

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005254771 A1 20051229 AU 2005-254771 20050614

CA 2568756 A1 20051229 CA 2005-2568756 20050614

EP 1761506 A1 20070314 EP 2005-752424 20050614

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV

NO 2007000199 A 20070111 NO 2007-199 20070111

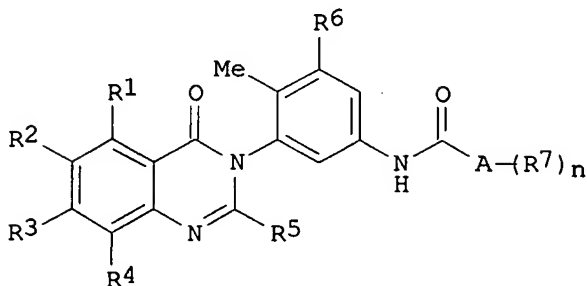
PRIORITY APPLN. INFO.:

US 2004-579265P P 20040615

WO 2005-GB2327 W 20050614

OTHER SOURCE(S): CASREACT 144:88308; MARPAT 144:88308

GI



I

AB Title compds. I [A = 5-6 membered carbocyclyl, 5-6 membered heterocyclyl; R1-6 = H, halo, NO₂, etc.; R7 = halo, NO₂, CN, OH, etc.; n = 1-4; with certain provisions] are prepared For instance, N-[3-(6-bromo-4-oxo-4H-quinazolin-3-yl)-4-methylphenyl]-3-trifluoromethylbenzamide is prepared from 2-amino-5-bromobenzoic acid, tri-Et orthoformate and N-(3-amino-4-methylphenyl)-3-trifluoromethylbenzamide (preparation given). Selected examples exhibit IC₅₀ in the range of 0.518 to 3.20 μM for B-Raf protein kinase. I are anticancer agents.

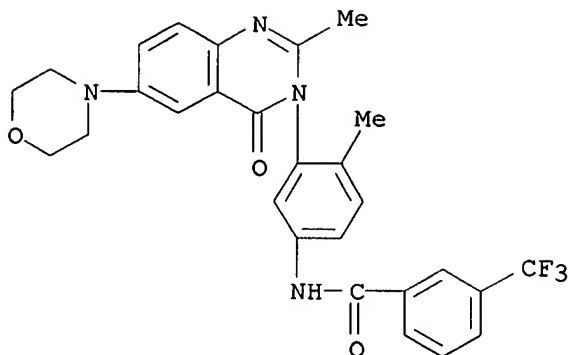
IT 872090-84-1P, N-[4-Methyl-3-[2-methyl-6-(morpholin-4-yl)-4-oxo-4H-quinazolin-3-yl]phenyl]-3-trifluoromethylbenzamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted quinazolones as B-Raf kinase inhibitors for treatment of cancer)

RN 872090-84-1 ZCAPLUS

CN Benzamide, N-[4-methyl-3-[2-methyl-6-(4-morpholinyl)-4-oxo-3(4H)-quinazolinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1324537 ZCAPLUS

DOCUMENT NUMBER: 144:142006

TITLE: Identification and Biological Characterization of 6-Aryl-7-isopropylquinazolinones as Novel TRPV1 Antagonists that Are Effective in Models of Chronic Pain

AUTHOR(S): Culshaw, Andrew J.; Bevan, Stuart; Christiansen, Martin; Copp, Prafula; Davis, Andrew; Davis, Clare; Dyson, Alex; Dziadulewicz, Edward K.; Edwards, Lee; Eggelte, Hendrikus; Fox, Alyson; Gentry, Clive; Groarke, Alex; Hallett, Allan; Hart, Terance W.; Hughes, Glyn A.; Knights, Sally; Kotsonis, Peter; Lee, Wai; Lyothier, Isabelle; McBryde, Andrew; McIntyre, Peter; Paloumbis, George; Panesar, Moh; Patel, Sadhana; Seiler, Max-Peter; Yaqoob, Mohammed; Zimmerman, Kaspar

CORPORATE SOURCE: Novartis Institutes for Biomedical Research, London, WC1E 6BS, UK

SOURCE: Journal of Medicinal Chemistry (2006), 49(2), 471-474
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:142006

AB Vanilloid receptor 1 (VR1, TRPV1) is a cation-selective ion channel that is expressed on primary afferent neurons and is upregulated following inflammation and nerve damage. Blockers of this channel may have utility in the treatment of chronic nociceptive and neuropathic pain. Here, we describe the optimization from a high throughput screening hit, of a series of 6-aryl-7-isopropylquinazolinones that are TRPV1 antagonists in vitro. We also demonstrate that one compound is active in vivo against capsaicin-induced hyperalgesia and in models of neuropathic and nociceptive pain in the rat.

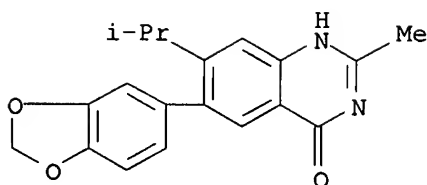
IT 681292-14-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(6-aryl-7-isopropylquinazolinones identification as TRPV1 antagonists, preparation and effect in chronic pain)

RN 681292-14-8 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-(1,3-benzodioxol-5-yl)-2-methyl-7-(1-methylethyl)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1144513 ZCAPLUS

DOCUMENT NUMBER: 144:36311

TITLE: Novel 7-methoxy-6-oxazol-5-yl-2,3-dihydro-1H-quinazolin-4-ones as IMPDH inhibitors

AUTHOR(S): Birch, Helen L.; Buckley, George M.; Davies, Natasha; Dyke, Hazel J.; Frost, Elizabeth J.; Gilbert, Philip J.; Hannah, Duncan R.; Haughan, Alan F.; Madigan, Michael J.; Morgan, Trevor; Pitt, William R.; Ratcliffe, Andrew J.; Ray, Nicholas C.; Richard, Marianna D.; Sharpe, Andrew; Taylor, Alicia J.; Whitworth, Justine M.; Williams, Sophie C.

CORPORATE SOURCE: UCB Celltech, Cambridge, CB1 6GS, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(23), 5335-5339

CODEN: BMCLE8; ISSN: 0960-894X

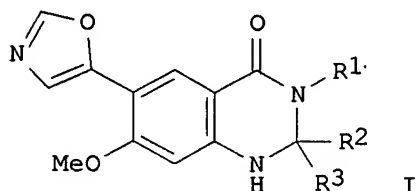
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:36311

GI



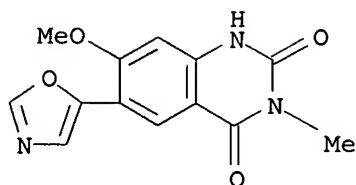
AB The synthesis and biol. activity of a novel series of 7-methoxy-6-oxazol-5-yl-2,3-dihydro-1H-quinazolin-4-ones I [R1 = Me, 2-(4-pyridyl)ethyl; R2 = Me, R3 = Me, PhCH:CH; R2R3 = (CH2)4, (CH2)2O(CH2)2, CH2N(CO2CMe3)CH2CH2, etc.] are described. Some of these compds. were found to be potent inhibitors of IMP dehydrogenase type II (IMPDH II).

IT 847941-19-9

RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of methoxy(oxazolyl)dihydroquinazolinones as IMP dehydrogenase inhibitors and antiproliferative agents)

RN 847941-19-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-4-one, 7-methoxy-3-methyl-6-(5-oxazolyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1021616 ZCAPLUS

DOCUMENT NUMBER: 143:326381

TITLE: Preparation of arylalkylamino-substituted quinazolines as type VR1 capsaicin receptor modulators

INVENTOR(S): Bakthavatchalam, Rajagopal; Chenard, Bertrand L.; Peterson, John M.; Steenstra, Cheryl K.

PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: PCT Int. Appl., 133 pp.

CODEN: PIXXD2

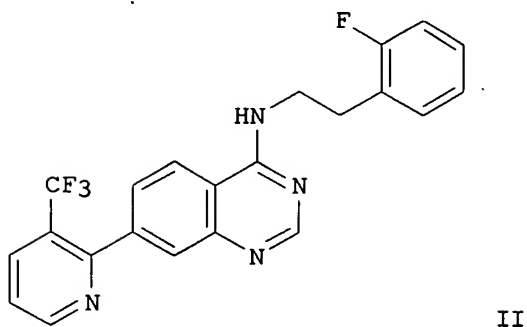
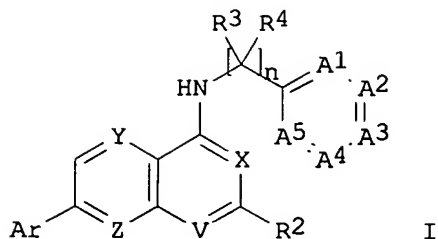
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087227	A1	20050922	WO 2005-US6697	20050301
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005221614	A1	20050922	AU 2005-221614	20050301
CA 2555867	A1	20050922	CA 2005-2555867	20050301
EP 1720542	A1	20061115	EP 2005-729370	20050301
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1950081	A	20070418	CN 2005-80014044	20050301
PRIORITY APPLN. INFO.:			US 2004-550216P	P 20040304
			WO 2005-US6697	W 20050301
OTHER SOURCE(S):	MARPAT 143:326381			
GI				



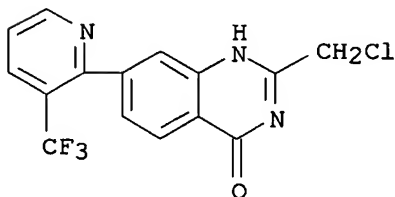
AB The title compds. I [V, X, Y and Z = N, CR1, such that at least one of V and X = N; R1 = H, halo, OH, etc.; R2 = halo, NO2, CN, etc.; n = 1-3; R3 = H, CN, alkyl, etc.; R4 = H, CN, alkyl; or R3 together with R4 forms an oxo group; or CR3R4 forms a 3-7 membered carbocycle or heterocycle; Ar = (un)substituted 5-10 membered carbocycle or heterocycle; A1 = N, CRa, or A1 is taken together with a R3 group to form an optionally substituted fused 5-7 membered carbocycle or heterocycle; A2-A5 = N, CRa; Ra = H, OH, halo, etc.] that are ligands that may be used to modulate specific receptor activity in vivo or in vitro, and are particularly useful in the treatment of conditions associated with pathol. receptor activation in humans, domesticated companion animals and livestock animals, were prepared. Thus, reacting 4-chloro-7-(3-trifluoromethylpyridin-2-yl)quinazolinone with 2-fluorophenethylamine afforded the quinazolinone II. The compds. I were tested in various tests for evaluating the VR1 modulator activity (data given). Pharmaceutical compns. and methods for using the compds. I to treat condition responsive to capsaicin receptor modulation are provided, as are methods for using such ligands for receptor localization studies.

IT 573680-42-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylalkylamino-substituted quinazolines as type VR1 capsaicin receptor modulators)

RN 573680-42-9 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-(chloromethyl)-7-[3-(trifluoromethyl)-2-pyridinyl]-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:979624 ZCAPLUS

DOCUMENT NUMBER: 143:286442

TITLE: Preparation of bicyclic pyrimidine derivatives as CCR4 function-controlling agents

INVENTOR(S): Kawano, Noriyuki; Igarashi, Susumu; Koganemaru, Yohei; Yamasaki, Shingo; Hattori, Kazuyuki; Masuda, Naoyuki; Ishikawa, Noriko; Miyazaki, Takahiro

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082865	A1	20050909	WO 2005-JP3207	20050225
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			JP 2004-53121	A 20040227
			JP 2004-183083	A 20040621
OTHER SOURCE(S):	MARPAT 143:286442			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = (un)substituted aryl, etc.; ring B = II, etc.; X = N, etc.; Y = N, etc.; Z = O, etc.; R1 = (un)substituted alkyl, etc.; R2 = halo, etc.; n = 0-3; m = 0-4; j = 0-3; k = 0-2] were prepared For example, reaction of 2-[(1'-{4-[(4-chlorophenyl)amino]-6,7-dimethoxyquinazolin-2-yl)-1,4'-bipiperidin-3-yl)methyl]-1H-isoindol-1,3(2H)-dione with hydrazine hydrate followed by treating with HCl afforded compound III·2HCl. In GTPγS binding assays, the IC50 value of compound III·2HCl was 13 nM. Compds. I are claimed useful for the treatment of inflammation, allergy, etc.

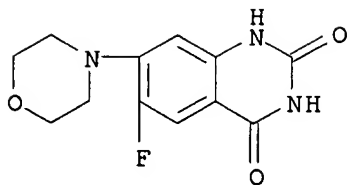
IT 769158-55-6P 864292-24-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bicyclic pyrimidine derivs. as CCR4 function-controlling agents for treatment of inflammation, allergy, etc.)

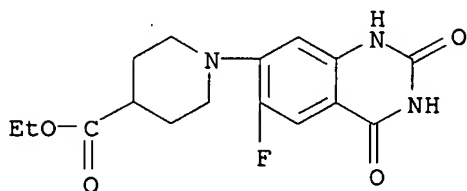
RN 769158-55-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-1-one, 6-fluoro-7-(4-morpholinyl)- (9CI) (CA INDEX NAME)



RN 864292-24-0 ZCAPLUS

CN 4-Piperidinecarboxylic acid, 1-(6-fluoro-1,2,3,4-tetrahydro-2,4-dioxo-7-quinazolinyl)-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:823314 ZCAPLUS

DOCUMENT NUMBER: 143:211923

TITLE: Preparation of fused-ring 4-oxopyrimidine derivatives as histamine H3 receptor antagonists or inverse agonists

INVENTOR(S): Nagase, Tsuyoshi; Sato, Nagaaki; Kanatani, Akio; Tokita, Shigeru

PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan

SOURCE: U.S. Pat. Appl. Publ., 84 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

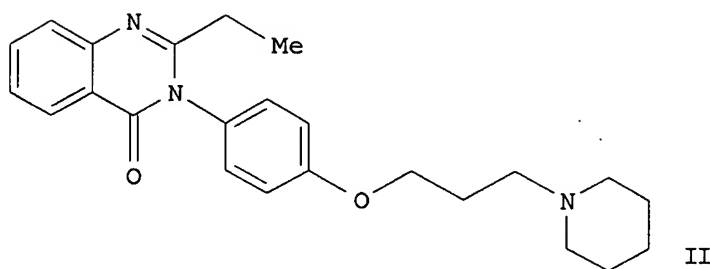
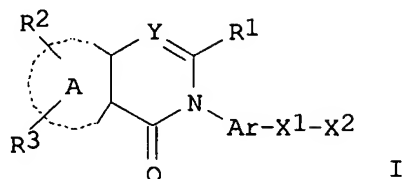
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005182045	A1	20050818	US 2005-58444	20050214
AU 2005212092	A1	20050825	AU 2005-212092	20050214
CA 2555824	A1	20050825	CA 2005-2555824	20050214
WO 2005077905	A1	20050825	WO 2005-JP2664	20050214
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1717230	A1	20061102	EP 2005-710446	20050214

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS
 CN 1918128 A 20070221 CN 2005-80004939 20050214
 NO 2006004089 A 20061106 NO 2006-4089 20060912
 PRIORITY APPLN. INFO.: JP 2004-37190 A 20040213
 WO 2005-JP2664 W 20050214

OTHER SOURCE(S): MARPAT 143:211923
 GI

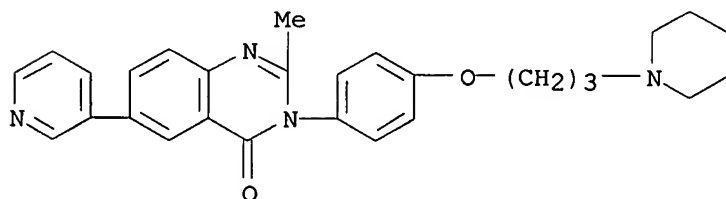


- AB The present invention provides fused-ring 4-oxopyrimidines (shown as I; variables defined below; e.g. 2-ethyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-4(3H)-quinazolinone (shown as II)) or pharmaceutically acceptable salts thereof, which, having histamine H3 receptor antagonist or inverse agonist activity, are useful in the prophylaxis or therapy of metabolic diseases, circulatory diseases, or nervous system diseases. For I: e.g. Ar is a divalent group formed by eliminating two H atoms from benzene; X1 = N, S, or O; R1 is a 5- to 6-membered heteroaryl group; Ring A is a 5- to 6-membered heteroaryl ring; R2 and R3 are amino or alkylamino groups; Y = CH or N; and X2 = -(CH2)_nNR4R5 (R4 and R5 are lower alkyl groups, and n = 2-4). Although the methods of preparation are not claimed, .apprx.275 example preps. are included. For example, II was prepared in 4 steps (98, 66, 82 and 47 %) starting from anthranilic acid and propionic anhydride and involving intermediates 2-ethyl-4H-3,1-benzoxazin-4-one, 2-ethyl-3-(4-hydroxyphenyl)-4(3H)-quinazolinone, and 2-ethyl-3-[4-(3-chloropropoxy)phenyl]-4(3H)-quinazolinone. Pharmacol. results are provided for II for the following tests: histamine analog coupling inhibition, antagonism of drinking behavior induced by R-α-methylhistamine (a histamine H3 receptor selective agonist), in vitro kinetics, and brain/cerebrospinal fluid activity.
- IT 862310-00-7P, 2-Methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(3-pyridyl)-4(3H)-quinazolinone 862310-02-9P, 2-Methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(4-pyridyl)-4(3H)-quinazolinone 862310-06-3P, 2-Methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(2-pyridyl)-4(3H)-quinazolinone
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of fused ring 4-oxopyrimidine derivs. as histamine H3 receptor antagonists or inverse agonists)

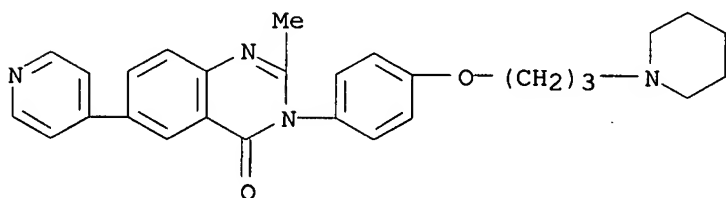
RN 862310-00-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(3-pyridinyl)- (9CI) (CA INDEX NAME)



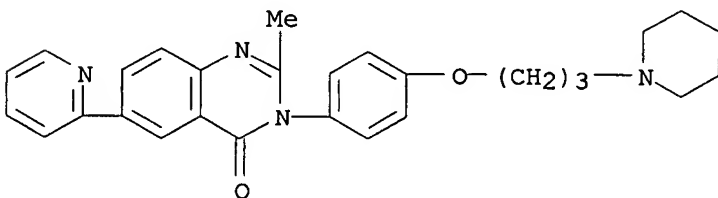
RN 862310-02-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 862310-06-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:300192 ZCAPLUS

DOCUMENT NUMBER: 142:373855

TITLE: Bis-quinazoline compounds for the treatment of bacterial infections and their preparation

INVENTOR(S): Guiles, Joseph; Dallmann, Garry; Janjic, Nebojsa; McHenry, Charles S.; Sun, Xicheng; Tregay, Ming

PATENT ASSIGNEE(S): Replidyne, Inc, USA

SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

WO 2005030131	A2	20050407	WO 2004-US31123	20040923
WO 2005030131	A3	20050512		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2005124562	A1	20050609	US 2004-948110	20040923
PRIORITY APPLN. INFO.:			US 2003-505524P	P 20030923
OTHER SOURCE(S):	CASREACT 142:373855; MARPAT 142:373855			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a group of bis-quinazoline compds. I, based on the compound (3,4-dihydroquinazolin-2-yl)-quinazolin-2-yl-amine, which are inhibitors of bacterial DNA polymerase holoenzymes. In compds. I, R2, R4, and R4' are independently selected from H, alkyl, alkenyl, alkynyl, arylmethyl, heterocyclomethyl, and Ph; R5, R5', R6, R6', R7, R7', R8, and R8' are independently selected from H, halo, nitro, cyano, OH, C1-7 alkyl, etc.; or a cyclic ring connecting any of: R5 and R6, R6 and R7, R7 and R8, R5' and R6', R6' and R7', and R7' and R8', where the cyclic ring is selected from (substituted) methylenedioxy, dioxane, 5-membered heterocycle, and 6-membered heterocycle; R6, R7, and R6' may also be various sidechains. The invention also relates to the preparation of I, pharmaceutical compns. containing I as active ingredients or pharmaceutically acceptable salts thereof, as well as to the use of the compns. for the treatment of bacterial infections. II, prepared by condensation of 2-amino-5-methoxyacetophenone HCl with sodium dicyanamide, was reacted with Et anthranilate to give bis-quinazoline III. The compds. of the invention have potent, reversible activity against DNA replication complexes from both Gram-pos. and Gram-neg. bacteria, with IC50 values ranging from <50 nM to 1 µM. At a dose of 25 mg/kg, IV was found to be non-toxic to mice and effective in protecting 50% of mice following infection with the min. LD of *S. aureus*.

IT 849423-33-2P, 2-(6,7-Dimethoxy-4-methylquinazolin-2-ylamino)-6-piperidin-1-ylquinazolin-4-ol trifluoroacetate 849423-35-4P, 2-(6,7-Dimethoxy-4-methylquinazolin-2-ylamino)-6-morpholin-4-ylquinazolin-4-ol trifluoroacetate

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of bis-quinazoline compds. for treatment of bacterial infections)

RN 849423-33-2 ZCAPLUS

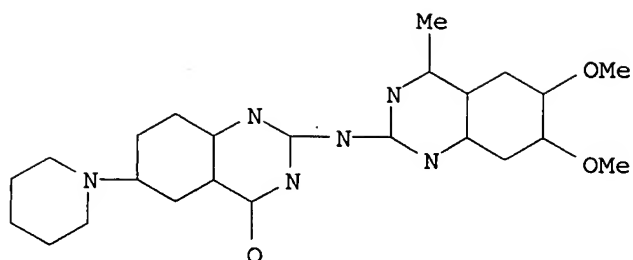
CN 4(1H)-Quinazolinone, 2-[(6,7-dimethoxy-4-methyl-2-quinazolinyl)amino]-6-(1-piperidinyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 849423-32-1

10/ 530,897

CMF C24 H26 N6 O3

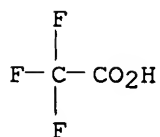


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1

CMF C2 H F3 O2



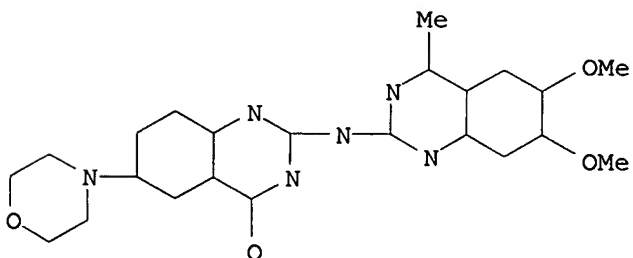
RN 849423-35-4 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[(6,7-dimethoxy-4-methyl-2-quinazolinyl)amino]-6-(4-morpholinyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 849423-34-3

CMF C23 H24 N6 O4

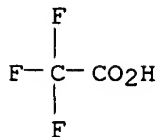


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

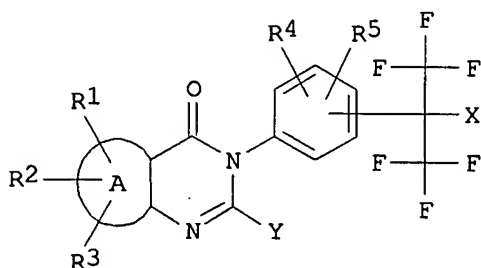
CRN 76-05-1

CMF C2 H F3 O2



L4 ANSWER 22 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:238967 ZCAPLUS
 DOCUMENT NUMBER: 142:316854
 TITLE: Preparation of substituted fused pyrimidine-4(3H)-one compounds with affinity for liver X receptors
 INVENTOR(S): Arai, Masami; Kaneko, Satoru; Shibuya, Satoshi; Watanabe, Tsuyoshi; Oda, Kozo
 PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan; X-Cepto Therapeutics, Inc.
 SOURCE: PCT Int. Appl., 406 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023782	A1	20050317	WO 2004-JP13268	20040906
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2006193426	A	20060727	JP 2003-314817	20030905
PRIORITY APPLN. INFO.:			JP 2003-314817	A 20030905
OTHER SOURCE(S):	MARPAT 142:316854			
GI				



I

AB The title compds. I [wherein ring A is Ph, etc.; R1 is R1a (R1a is substituted alkyl, etc.), Z1bR1b (R1b is substituted alkyl, etc. and Z1b is NH, etc.), etc.; R2 and R3 each is hydrogen, optionally substituted alkyl, OH, etc.; R4 and R5 each is hydrogen, optionally substituted alkyl,

OH, etc.; X is OH or alkoxy; and Y is optionally substituted alkyl, etc., provided that when Y is a specific group and A is Ph, then R₄ and R₅ each is hydrogen and C(CF₃)₂(X) is C(CF₃)₂(OH) bonded to the Ph group in the 3- or 4-position thereof] are prepared. Thus, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(3-pyridylmethyl)-6-(3-thienyl)-4-(3H)-quinazolinone was prepared from 6-iodo-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(3-pyridylmethyl)-4-(3H)-quinazolinone and 3-thienylboronic acid. In an in vitro assay for affinity for the LXR α and LXR β receptors, compds. of this invention showed K_i values of $\leq 1 \mu\text{M}$. I are useful for the treatment of arteriosclerosis, hyperlipemia, inflammatory diseases, etc. Formulations are given.

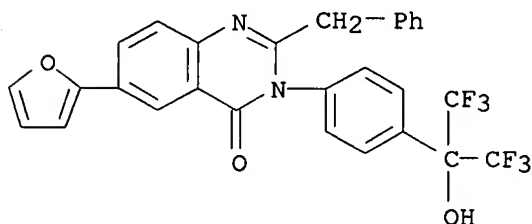
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 848093-59-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted fused pyrimidine-4(3H)-one compds. with affinity for liver X receptors)

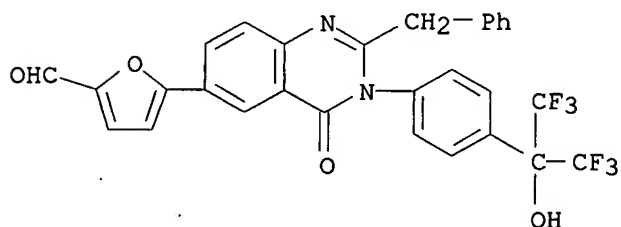
RN 848089-84-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(2-furanyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



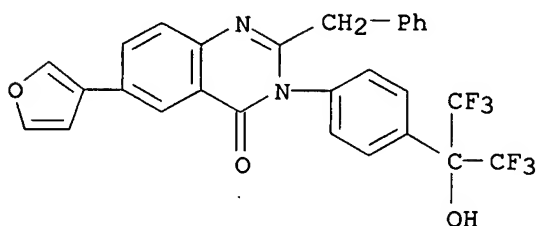
RN 848089-85-0 ZCAPLUS

CN 2-Furancarboxaldehyde, 5-[3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-quinazolinyl]- (9CI) (CA INDEX NAME)



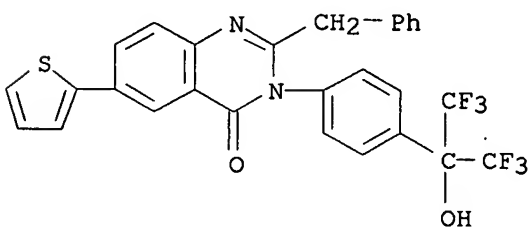
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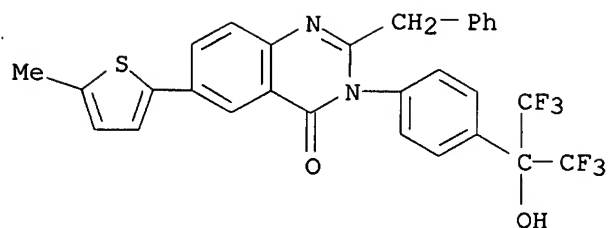
RN 848089-87-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(2-thienyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



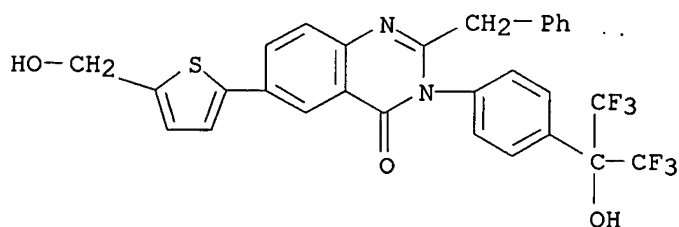
RN 848089-88-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(5-methyl-2-thienyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



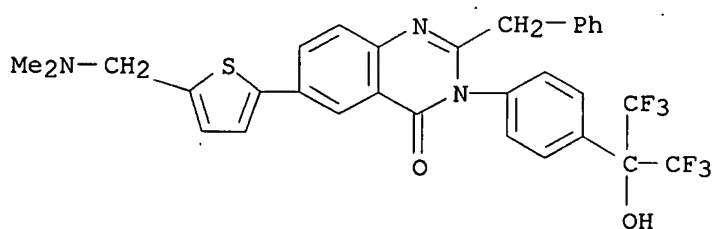
RN 848089-89-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-[5-(hydroxymethyl)-2-thienyl]-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



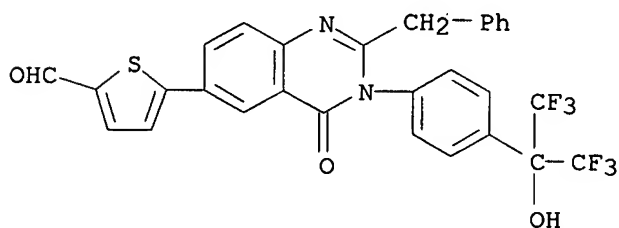
RN 848089-90-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-[5-[(dimethylamino)methyl]-2-thienyl]-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848089-91-8 ZCAPLUS

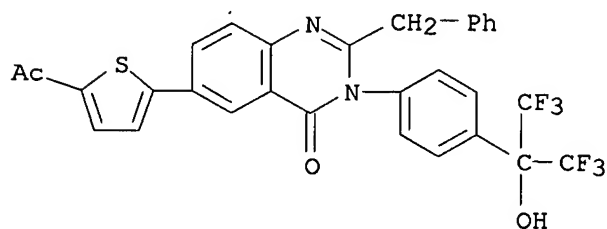
CN 2-Thiophenecarboxaldehyde, 5-[3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 848089-92-9 ZCAPLUS

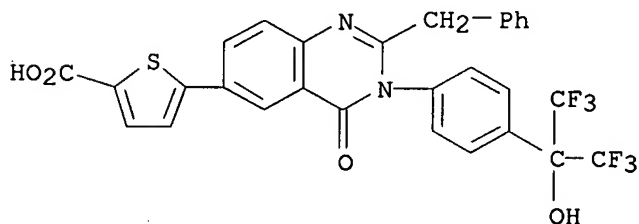
CN 4(3H)-Quinazolinone, 6-(5-acetyl-2-thienyl)-2-(phenylmethyl)-3-[4-[2,2,2-

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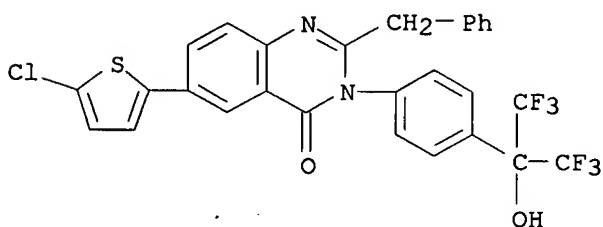
RN 848089-93-0 ZCAPLUS

CN 2-Thiophenecarboxylic acid, 5-[3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-quinazolinyl]- (9CI) (CA INDEX NAME)



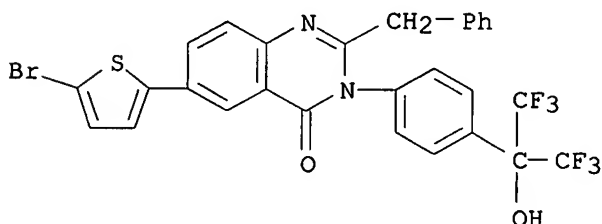
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CN 4(3H)-Quinazolinone, 6-(5-chloro-2-thienyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



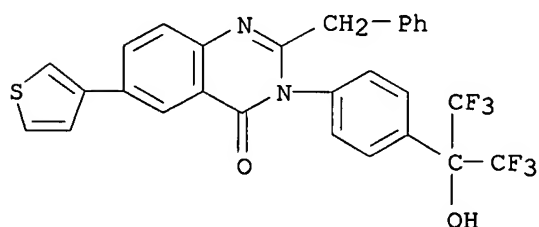
RN 848089-95-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(5-bromo-2-thienyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



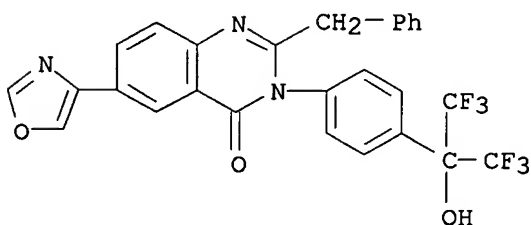
RN 848089-96-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(3-thienyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



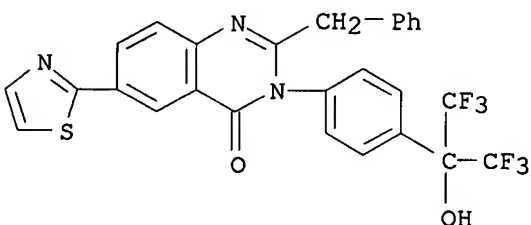
RN 848089-99-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(4-oxazolyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



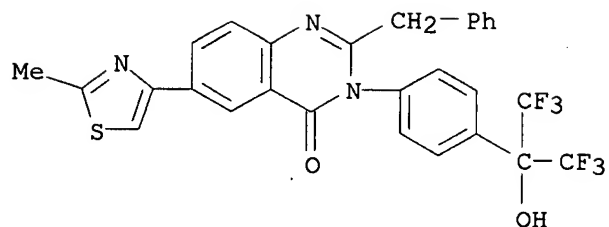
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CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(2-thiazolyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



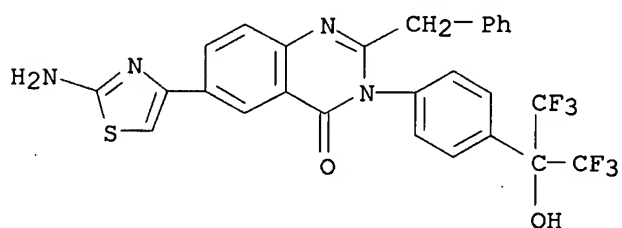
RN 848090-01-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(2-methyl-4-thiazolyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



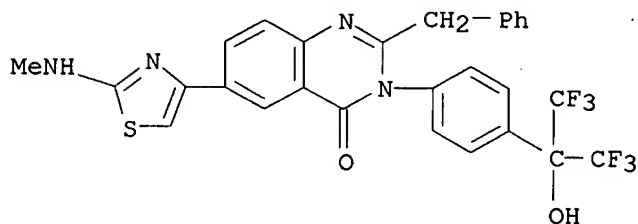
RN 848090-02-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(2-amino-4-thiazolyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



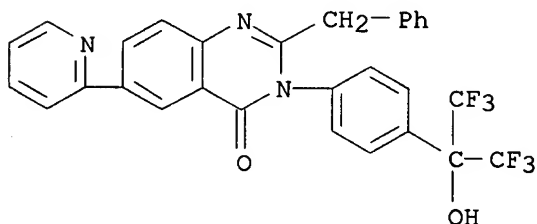
RN 848090-03-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-[2-(methylamino)-4-thiazolyl]-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848090-05-1 ZCAPLUS

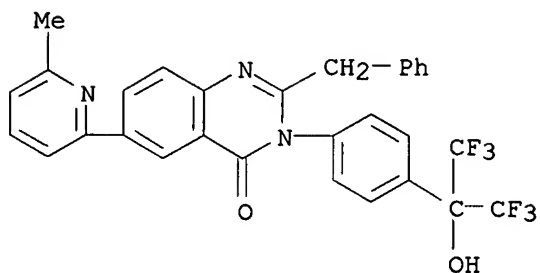
CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848090-06-2 ZCAPLUS

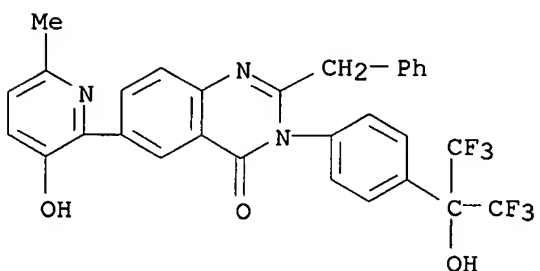
CN 4(3H)-Quinazolinone, 6-(6-methyl-2-pyridinyl)-2-(phenylmethyl)-3-[4-[2,2,2-

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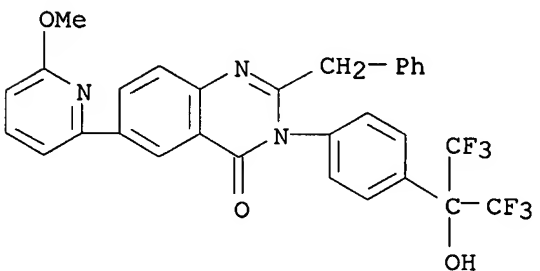
RN 848090-07-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(3-hydroxy-6-methyl-2-pyridinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



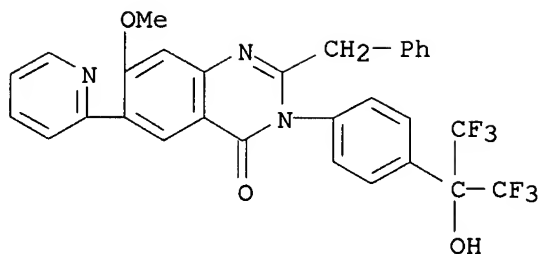
RN 848090-08-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(6-methoxy-2-pyridinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



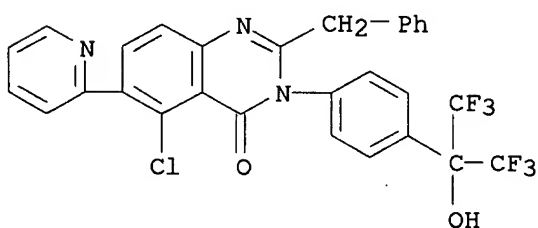
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CN 4(3H)-Quinazolinone, 7-methoxy-2-(phenylmethyl)-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



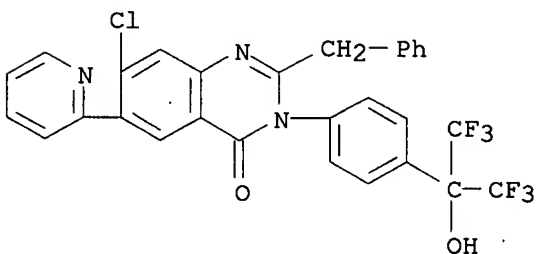
RN 848090-10-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 5-chloro-2-(phenylmethyl)-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



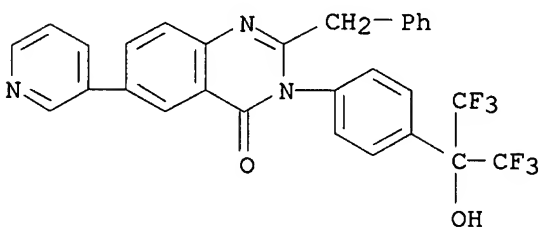
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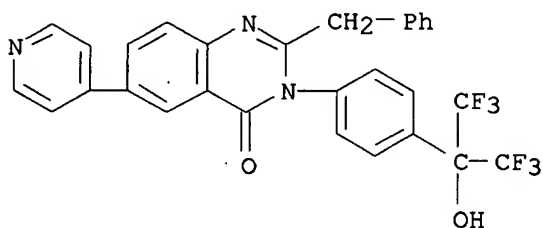
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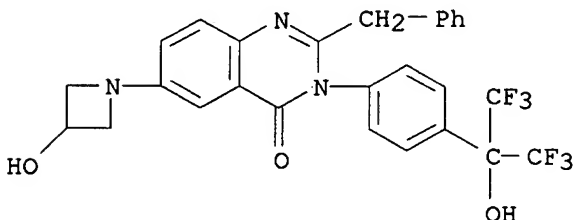
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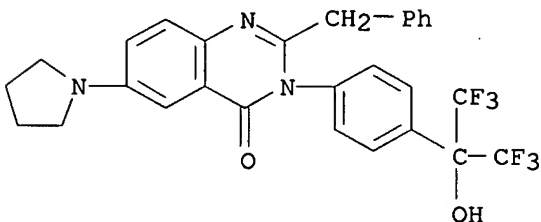
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CN 4(3H)-Quinazolinone, 6-(3-hydroxy-1-azetidiny)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



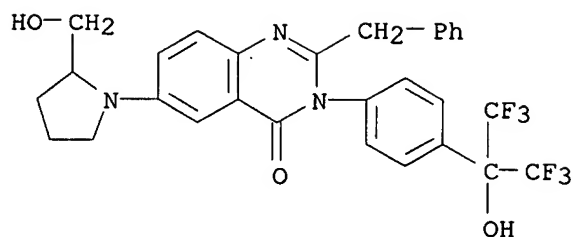
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CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(1-pyrrolidinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



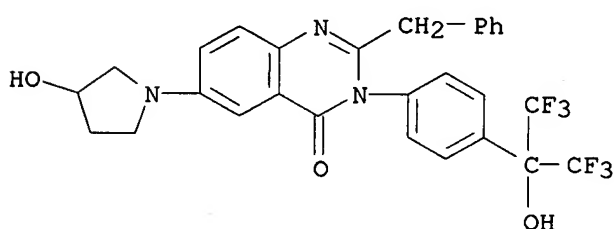
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CN 4(3H)-Quinazolinone, 6-[2-(hydroxymethyl)-1-pyrrolidinyl]-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



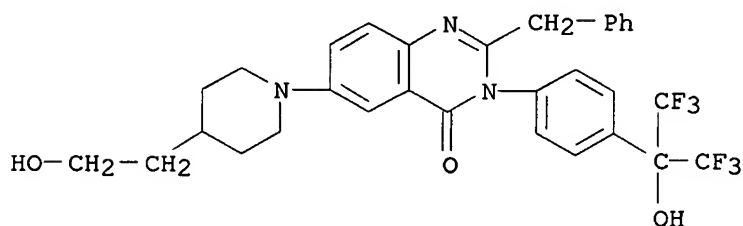
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CN 4(3H)-Quinazolinone, 6-(3-hydroxy-1-pyrrolidinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



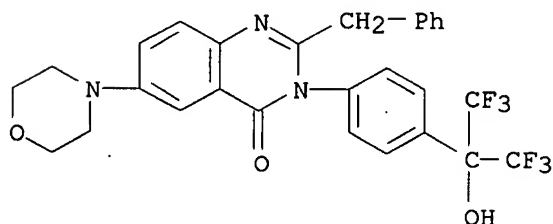
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RN 848090-19-7 ZCAPLUS

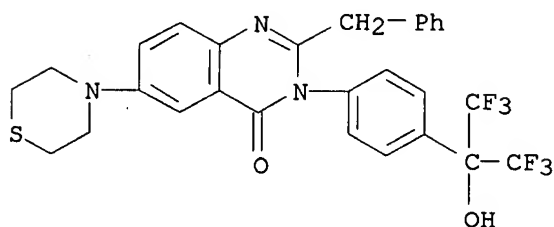
CN 4(3H)-Quinazolinone, 6-(4-morpholinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848090-20-0 ZCAPLUS

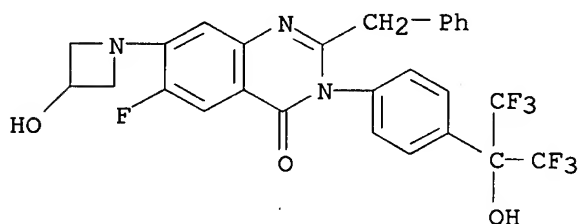
CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(4-thiomorpholinyl)-3-[4-[2,2,2-

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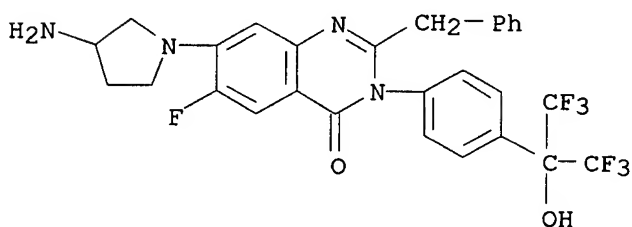
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CN 4(3H)-Quinazolinone, 6-fluoro-7-(3-hydroxy-1-azetidiny)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



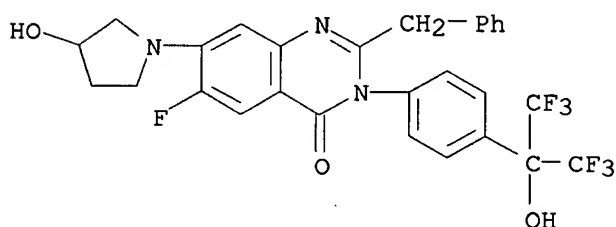
RN 848090-24-4 ZCAPLUS

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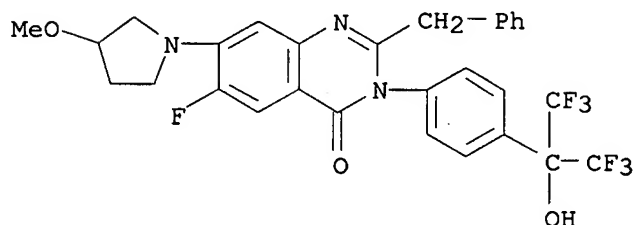
RN 848090-25-5 ZCAPLUS

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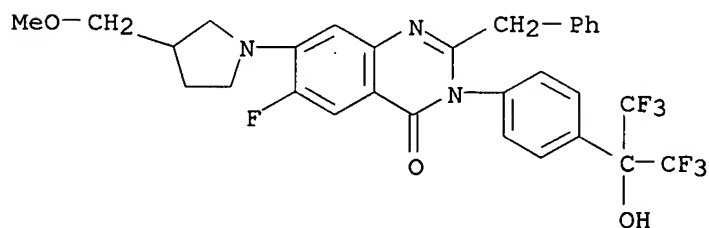
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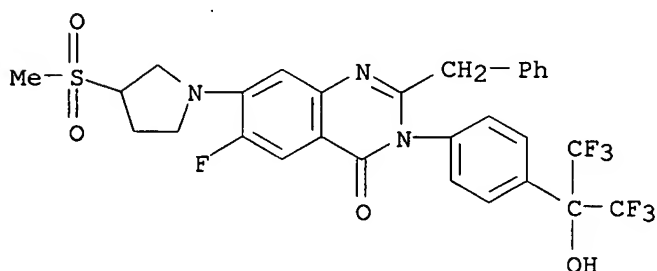
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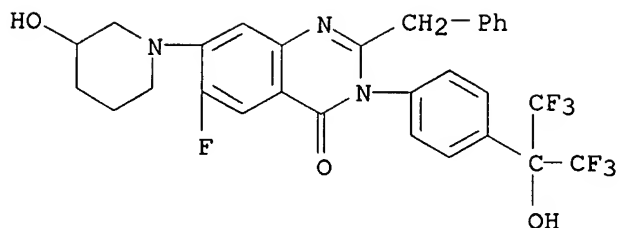
RN 848090-28-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-7-[3-(methylsulfonyl)-1-pyrrolidinyl]-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



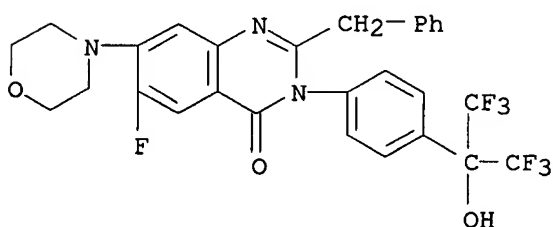
RN 848090-29-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-7-(3-hydroxy-1-piperidinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



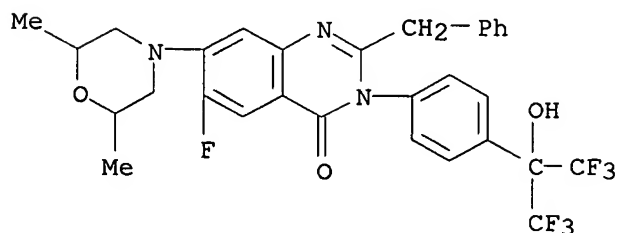
RN 848090-30-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-7-(4-morpholinyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



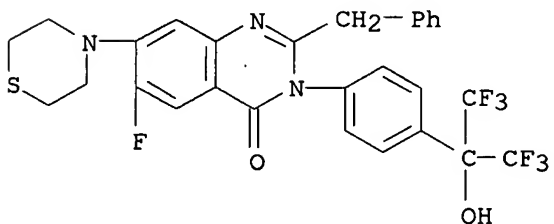
RN 848090-31-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 7-(2,6-dimethyl-4-morpholinyl)-6-fluoro-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848090-34-6 ZCAPLUS

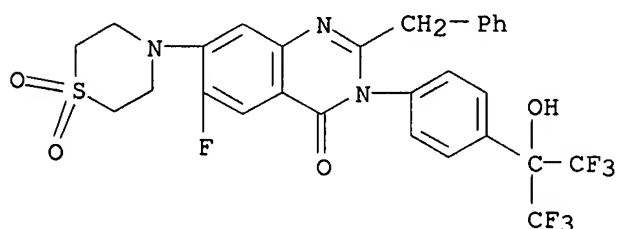
CN 4(3H)-Quinazolinone, 6-fluoro-2-(phenylmethyl)-7-(4-thiomorpholinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848090-35-7 ZCAPLUS

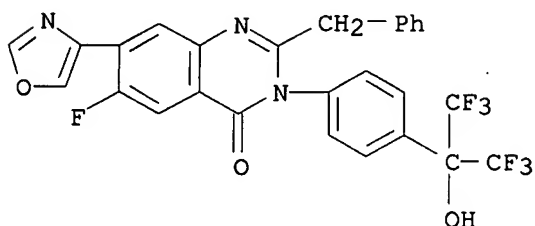
CN 4(3H)-Quinazolinone, 7-(1,1-dioxido-4-thiomorpholinyl)-6-fluoro-2-

(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



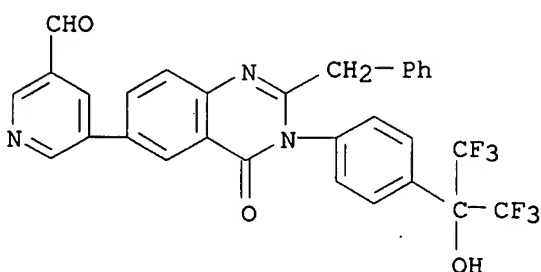
RN 848090-36-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-7-(4-oxazolyl)-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



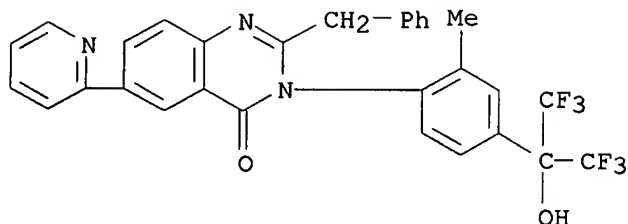
RN 848090-38-0 ZCAPLUS

CN 3-Pyridinecarboxaldehyde, 5-[3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-quinazolinyl]- (9CI) (CA INDEX NAME)



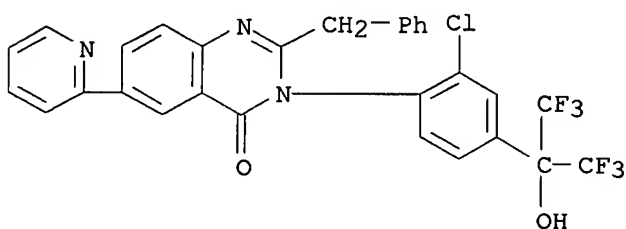
RN 848091-23-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



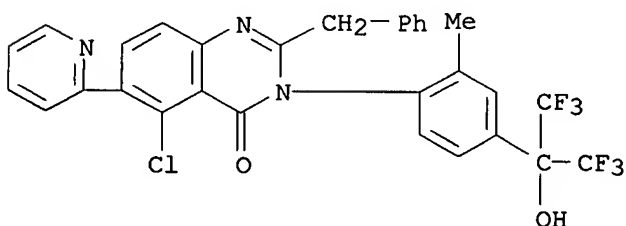
RN 848091-24-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-chloro-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI)
(CA INDEX NAME)



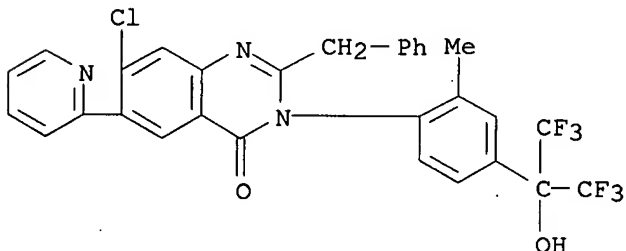
RN 848091-25-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 5-chloro-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI)
(CA INDEX NAME)



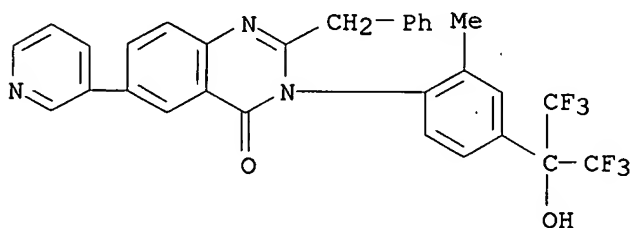
RN 848091-26-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 7-chloro-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI)
(CA INDEX NAME)



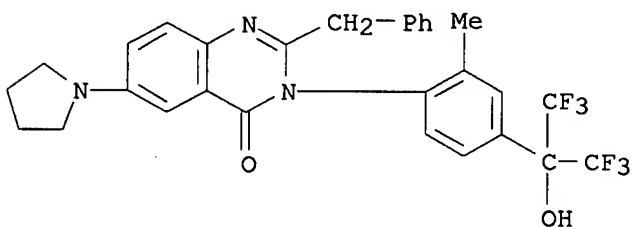
RN 848091-27-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(3-pyridinyl)- (9CI)
(CA INDEX NAME)



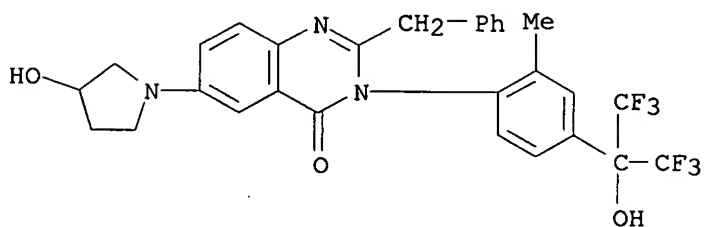
RN 848091-29-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(1-pyrrolidinyl)- (9CI)
(CA INDEX NAME)



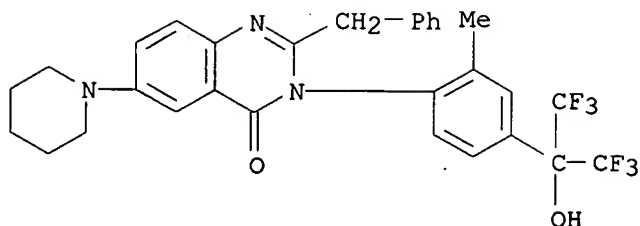
RN 848091-30-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(3-hydroxy-1-pyrrolidinyl)-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



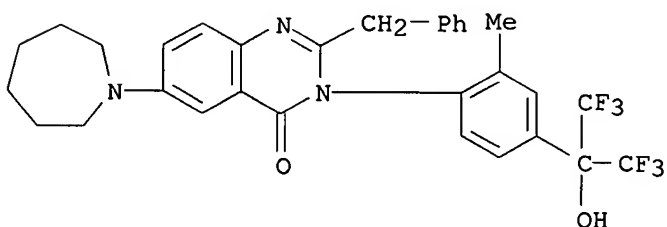
RN 848091-31-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(1-piperidinyl)- (9CI)
(CA INDEX NAME)



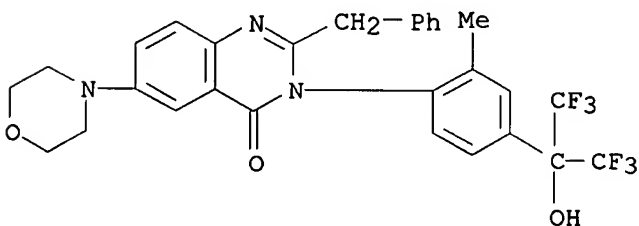
RN 848091-32-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(hexahydro-1H-azepin-1-yl)-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



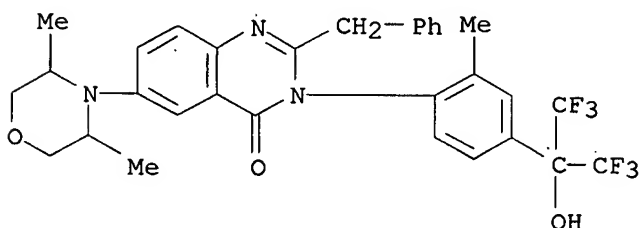
RN 848091-33-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(4-morpholinyl)-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 848091-34-9 ZCAPLUS

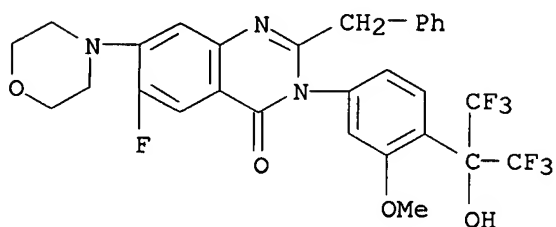
CN 4(3H)-Quinazolinone, 6-(3,5-dimethyl-4-morpholinyl)-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 848091-40-7 ZCAPLUS

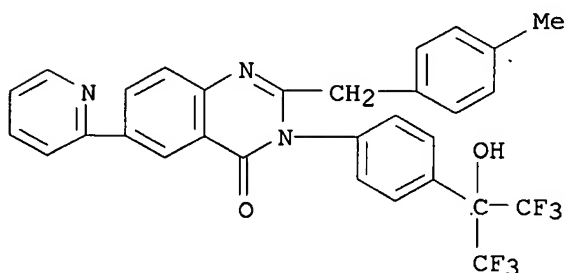
CN 4(3H)-Quinazolinone, 6-fluoro-3-[3-methoxy-4-[2,2,2-trifluoro-1-hydroxy-1-

(trifluoromethyl)ethyl]phenyl]-7-(4-morpholinyl)-2-(phenylmethyl)- (9CI)
(CA INDEX NAME)



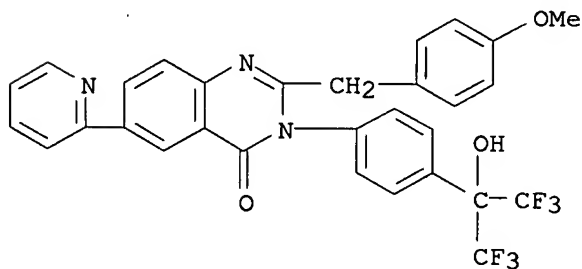
RN 848091-54-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(4-methylphenyl)methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



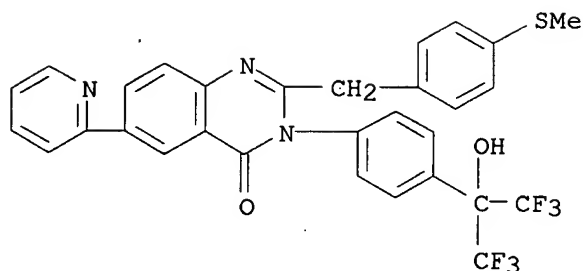
RN 848091-55-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(4-methoxyphenyl)methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



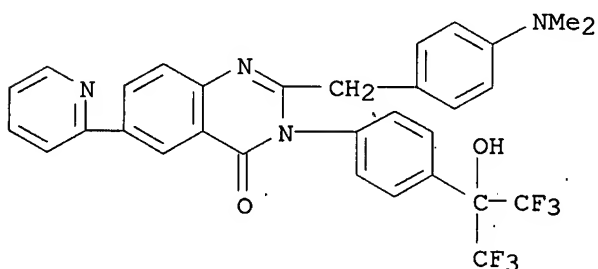
RN 848091-56-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[[4-(methylthio)phenyl]methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



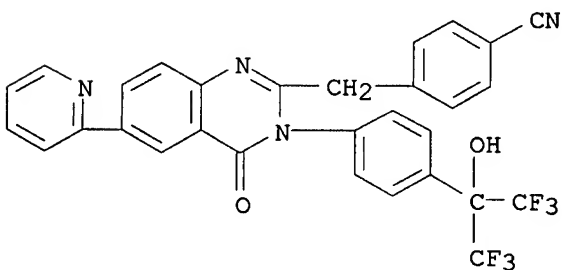
RN 848091-57-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[[4-(dimethylamino)phenyl]methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



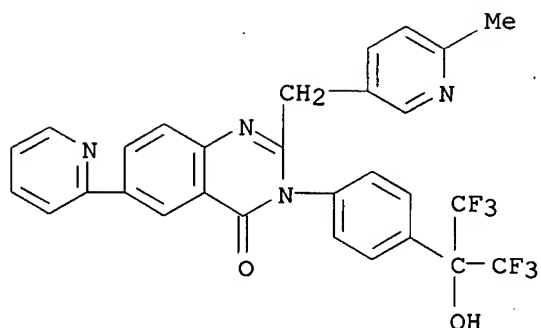
RN 848091-58-7 ZCAPLUS

CN Benzonitrile, 4-[[[3,4-dihydro-4-oxo-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



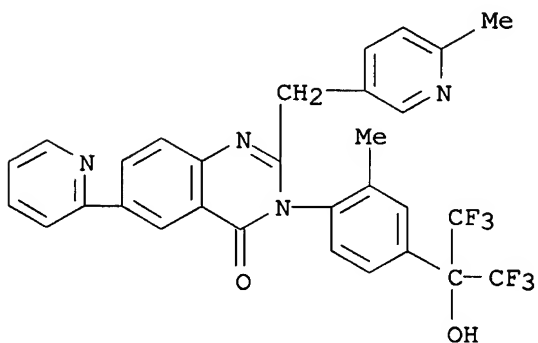
RN 848091-59-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(6-methyl-3-pyridinyl)methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



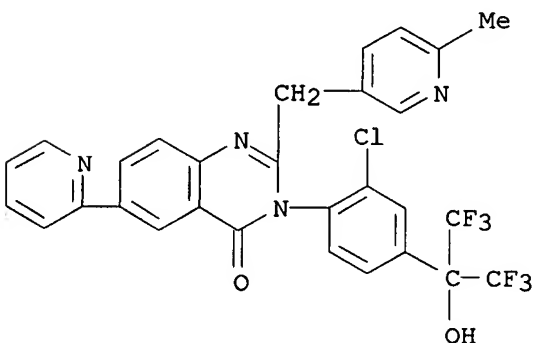
RN 848091-60-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(6-methyl-3-pyridinyl)methyl]-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



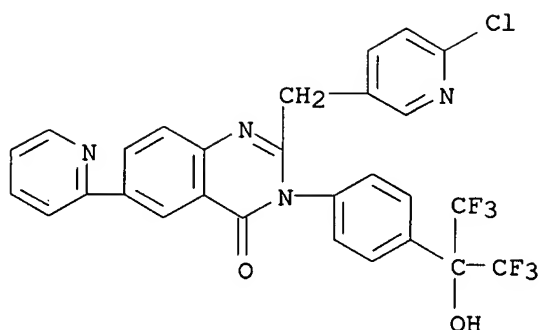
RN 848091-61-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-chloro-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-[(6-methyl-3-pyridinyl)methyl]-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



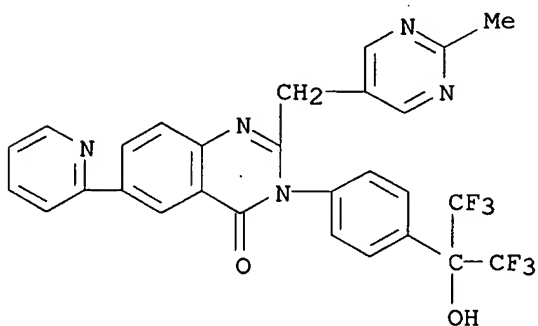
RN 848091-63-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(6-chloro-3-pyridinyl)methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



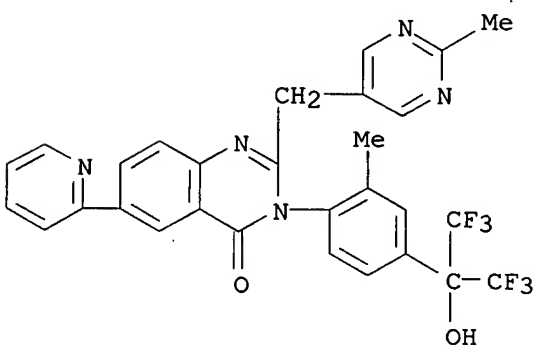
RN 848091-64-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(2-methyl-5-pyrimidinyl)methyl]-6-(2-pyridinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



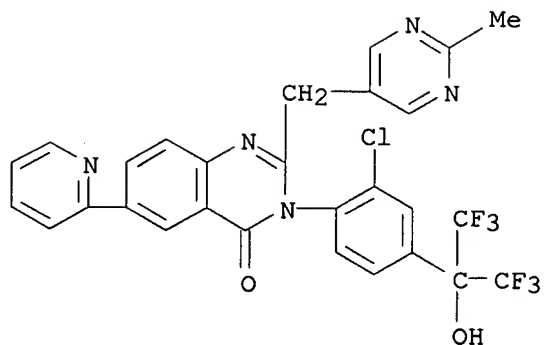
RN 848091-65-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(2-methyl-5-pyrimidinyl)methyl]-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



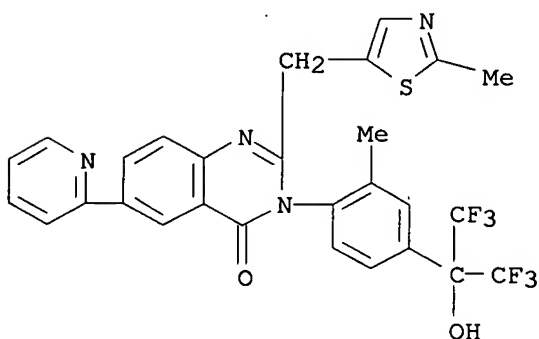
RN 848091-66-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-chloro-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-[(2-methyl-5-pyrimidinyl)methyl]-6-(2-pyridinyl)- (9CI) (CA INDEX NAME)



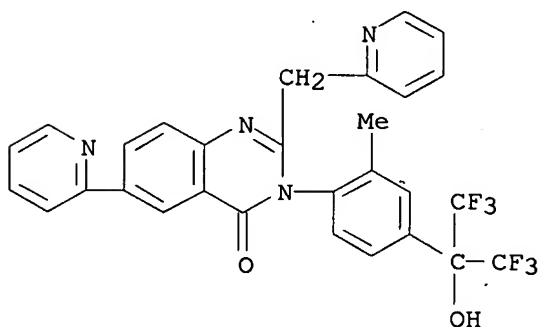
RN 848091-68-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-[(2-methyl-5-thiazolyl)methyl]-3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)-
(9CI) (CA INDEX NAME)



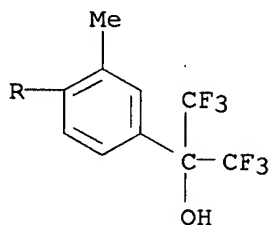
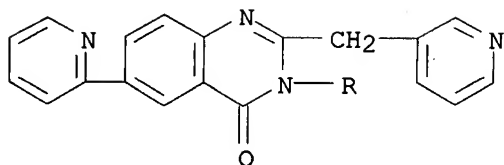
RN 848091-69-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)-2-(2-pyridinylmethyl)-
(9CI) (CA INDEX NAME)

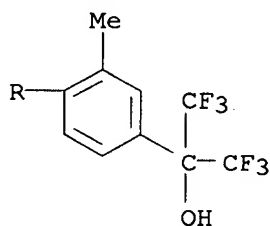
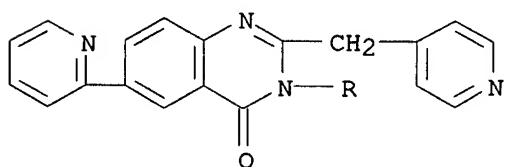


RN 848091-70-3 ZCAPLUS

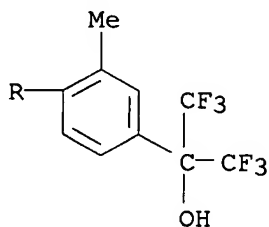
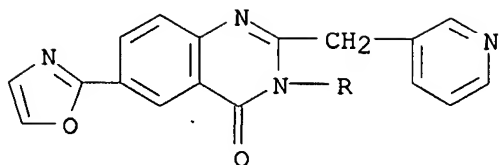
CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)-2-(3-pyridinylmethyl)-
(9CI) (CA INDEX NAME)



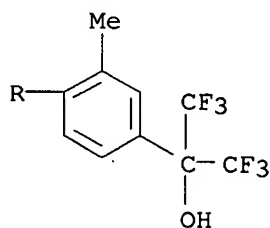
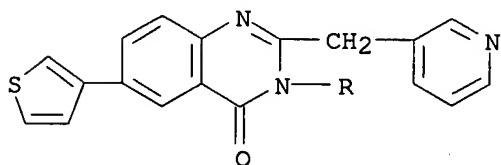
RN 848091-71-4 ZCAPLUS
 CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-pyridinyl)-2-(4-pyridinylmethyl)-(9CI) (CA INDEX NAME)



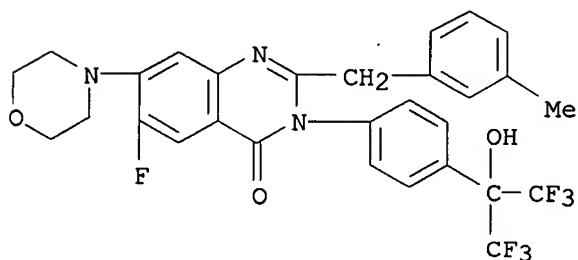
RN 848092-14-8 ZCAPLUS
 CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-(2-oxazolyl)-2-(3-pyridinylmethyl)-(9CI) (CA INDEX NAME)



RN 848092-15-9 ZCAPLUS
 CN 4(3H)-Quinazolinone, 3-[2-methyl-4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(3-pyridinylmethyl)-6-(3-thienyl)- (9CI)
 (CA INDEX NAME)

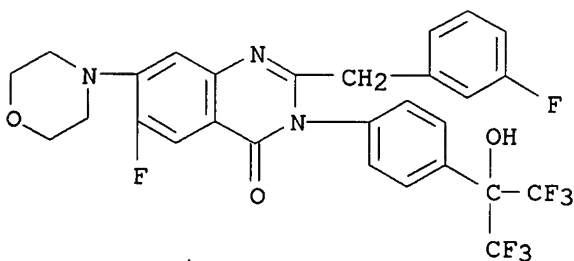


RN 848092-17-1 ZCAPLUS
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 (CA INDEX NAME)

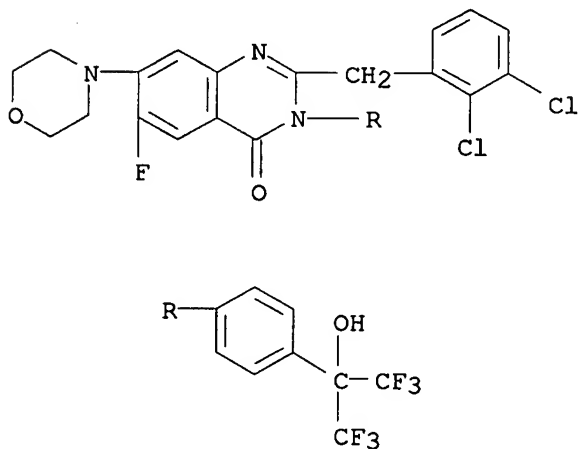


RN 848092-18-2 ZCAPLUS

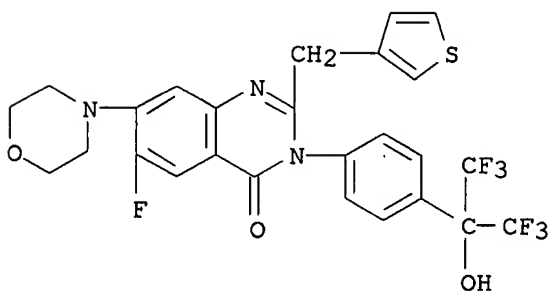
CN 4(3H)-Quinazolinone, 6-fluoro-2-[(3-fluorophenyl)methyl]-7-(4-morpholinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI)
(CA INDEX NAME)



RN 848092-19-3 ZCAPLUS
CN 4(3H)-Quinazolinone, 2-[(2,3-dichlorophenyl)methyl]-6-fluoro-7-(4-morpholinyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

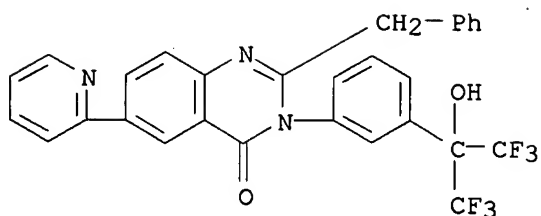


RN 848092-20-6 ZCAPLUS
CN 4(3H)-Quinazolinone, 6-fluoro-7-(4-morpholinyl)-2-(3-thienylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



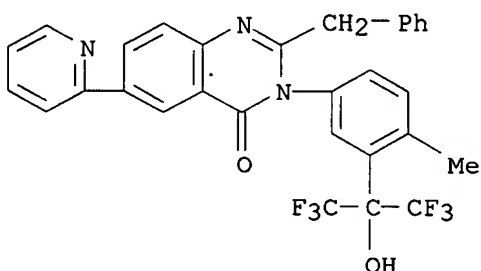
RN 848092-29-5 ZCAPLUS
CN 4(3H)-Quinazolinone, 2-(phenylmethyl)-6-(2-pyridinyl)-3-[3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

NAME)



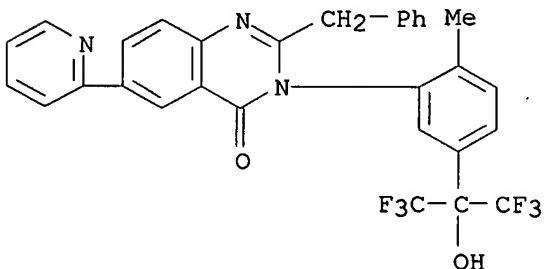
RN 848092-30-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[4-methyl-3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI)
(CA INDEX NAME)



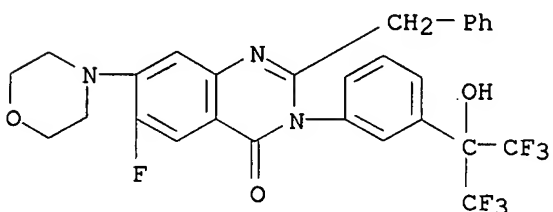
RN 848092-31-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-[2-methyl-5-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-2-(phenylmethyl)-6-(2-pyridinyl)- (9CI)
(CA INDEX NAME)

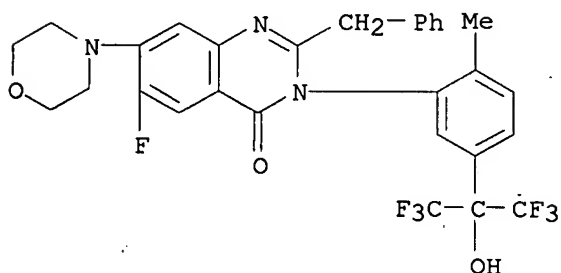


RN 848092-33-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-7-(4-morpholinyl)-2-(phenylmethyl)-3-[3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

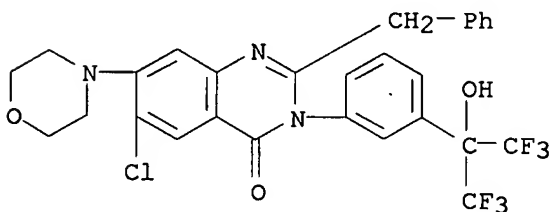


RN 848092-34-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-fluoro-3-[2-methyl-5-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-7-(4-morpholinyl)-2-(phenylmethyl)- (9CI)
(CA INDEX NAME)

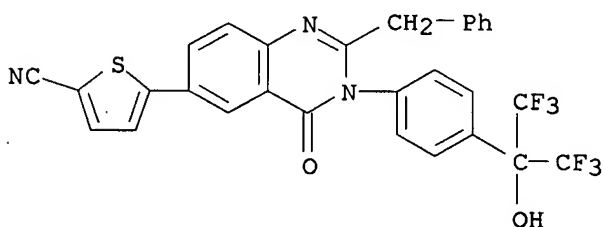
RN 848092-42-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-chloro-7-(4-morpholinyl)-2-(phenylmethyl)-3-[3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)



RN 848093-59-4 ZCAPLUS

CN 2-Thiophenecarbonitrile, 5-[3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-6-quinazolinyl]- (9CI) (CA INDEX NAME)



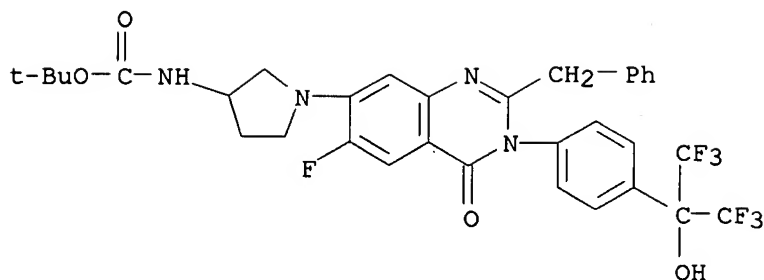
IT 848093-08-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted fused pyrimidine-4(3H)-one compds. with affinity for liver X receptors)

RN 848093-08-3 ZCAPLUS

CN Carbamic acid, [1-[6-fluoro-3,4-dihydro-4-oxo-2-(phenylmethyl)-3-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]-7-quinazolinyl]-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:232568 ZCAPLUS

DOCUMENT NUMBER: 142:291383

TITLE: Nitrosated and nitrosylated cardiovascular compounds, compositions, and methods of therapeutic use

INVENTOR(S): Garvey, David S.; Letts, Gordon L.; Worcel, Manuel

PATENT ASSIGNEE(S): Nitromed, Inc., USA

SOURCE: PCT Int. Appl., 126 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023182	A2	20050317	WO 2004-US26910	20040820
WO 2005023182	A3	20061019		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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AU 2004270162	A1	20050317	AU 2004-270162	20040820
CA 2536967	A1	20050317	CA 2004-2536967	20040820
CA 2536975	A1	20050317	CA 2004-2536975	20040820
US 2005059655	A1	20050317	US 2004-921936	20040820
WO 2005023183	A2	20050317	WO 2004-US26911	20040820
WO 2005023183	A3	20051013		
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SN, TD, TG
 EP 1667643 A2 20060614 EP 2004-781570 20040820
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 EP 1668008 A2 20060614 EP 2004-781571 20040820
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 JP 2007504135 T 20070301 JP 2006-524730 20040820
 JP 2007504136 T 20070301 JP 2006-524731 20040820
 PRIORITY APPLN. INFO.: US 2003-498309P P 20030828
 US 2004-535542P P 20040112
 WO 2004-US26910 W 20040820
 WO 2004-US26911 W 20040820

OTHER SOURCE(S): MARPAT 142:291383

AB The invention provides nitrosated and/or nitrosylated cardiovascular compds. or pharmaceutically acceptable salts thereof, and compns. comprising at least one nitrosated and/or nitrosylated cardiovascular compound, and, optionally, at least one nitric oxide donor and/or at least one therapeutic agent. The invention also provides compns. and kits comprising at least one cardiovascular compound of the invention that is optionally nitrosated and/or nitrosylated and, optionally, at least one nitric oxide donor compound and/or at least one therapeutic agent. The invention also provides methods for (a) treating cardiovascular diseases; (b) treating renovascular diseases; (c) treating diabetes; (d) treating diseases resulting from oxidative stress; (e) treating endothelial dysfunctions; (f) treating diseases caused by endothelial dysfunctions; (g) treating cirrhosis; (h) treating pre-eclampsia; (j) treating osteoporosis; and (k) treating nephropathy. The nitrosated and/or nitrosylated cardiovascular compds. are preferably nitrosated and/or nitrosylated aldosterone antagonists, nitrosated and/or nitrosylated angiotensin II antagonists, nitrosated and/or nitrosylated calcium channel blockers, nitrosated and/or nitrosylated endothelin antagonists, nitrosated and/or nitrosylated hydralazine compds., nitrosated and/or nitrosylated neutral endopeptidase inhibitors and nitrosated and/or nitrosylated renin inhibitors.

IT 167301-42-0D, nitrosated/nitrosylated derivs.

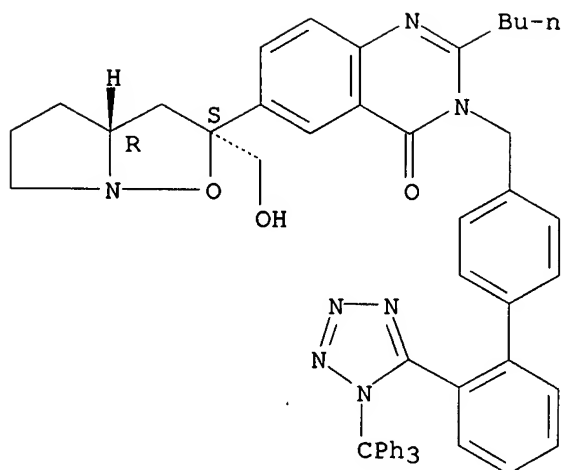
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(nitrosated and nitrosylated cardiovascular compds., compns., and therapeutic use)

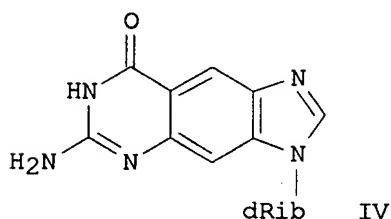
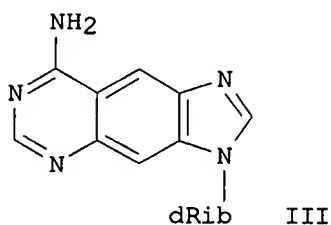
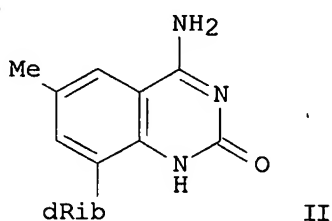
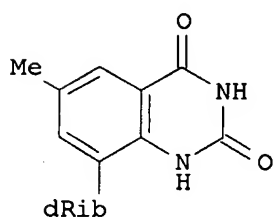
RN 167301-42-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[(2R,3aS)-hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 24 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:200901 ZCAPLUS
 DOCUMENT NUMBER: 143:320146
 TITLE: Design of size-expanded genetic systems
 AUTHOR(S): Kool, Eric T.
 CORPORATE SOURCE: Department of Chemistry, Stanford University,
 Stanford, CA, 94305, USA
 SOURCE: Polymer Preprints (American Chemical Society, Division
 of Polymer Chemistry) (2005), 46(1), 133-134
 CODEN: ACPPAY; ISSN: 0032-3934
 PUBLISHER: American Chemical Society, Division of Polymer
 Chemistry
 DOCUMENT TYPE: Journal; (computer optical disk)
 LANGUAGE: English
 GI



AB In this paper we describe design principles for a different approach to genetic biopolymers, in which we construct new base pairs for a

non-natural DNA-like paired helix. The present approach involves benzohomologated deoxyribosides, denoted dxT, dxC, dxA, and dxG (I-IV, resp.; dRib = 2'-deoxy- β -D-ribose), which have bases that are larger than the natural ones by 2.4 Å, the width of a benzene ring. When paired with natural partners, these form base pairs that are expanded by this length. If all base pairs are expanded in an analogous way, this creates an expanded double helix, termed xDNA. xDNA has the potential to encode more information than the natural genetic system. Here we describe structural comparisons of purines and pyrimidines for this artificial genetic encoding helix, and we analyze conformational adjustments to the phosphodiester backbone that are needed to accept such a dimensional change. We further propose the possibility of further expansion of such a helix. Finally, we discuss possible biol. and biomedical implications of this designed genetic system.

IT 639465-38-6

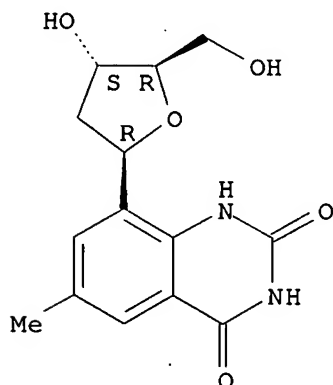
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(dxT; design of expanded genetic systems using benzo-expanded nucleic acid bases)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-6-one, 8-(2-deoxy- β -D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry:



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:139452 ZCAPLUS

DOCUMENT NUMBER: 142:406141

TITLE: A New Four-Base Genetic Helix, yDNA, Composed of Widened Benzopyrimidine-Purine Pairs

AUTHOR(S): Lee, Alex H. F.; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA

SOURCE: Journal of the American Chemical Society (2005), 127(10), 3332-3338

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

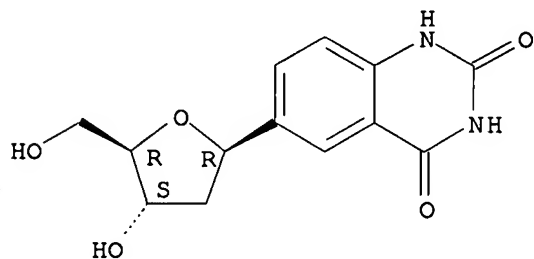
LANGUAGE: English

AB We describe the properties of stable DNA-like self-assembled helices composed entirely of base pairs involving two new size-expanded pyrimidines. We term this new helix geometry "yDNA" (an abbreviation of

"wide DNA"). The new pyrimidine analogs, yT and yC, are increased in size by benzo-homologation and have a geometry that is distinct from previous size-expanded pyrimidines. The yT and yC deoxyribosides were incorporated into oligodeoxynucleotides designed to form four pairs: yT-A, A-yT, yC-G, and G-yC. Helixes were characterized by thermal denaturation, mixing data, and CD spectra. Results showed that highly stable double-stranded helixes were formed in several sequence contexts. The data further showed that yT and yC could be segregated onto one strand and used to bind to natural strands of DNA with high sequence selectivity. The combination of yC, yT, G, and A make up a new selective, self-assembling four-base genetic pairing system that functions in many respects like natural DNA, but which is structurally distinct. The results establish that multiple variants of size-expanded DNA-like helixes are feasible and suggest the possibility of a future eight-base genetic system based on the yDNA geometry. Finally, the high binding selectivity, affinity, and fluorescence of yDNA strands may yield useful applications in detection of nucleic acid sequences.

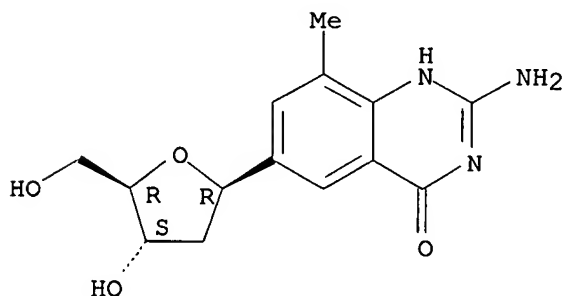
IT 830343-25-4D, base pairing with adenine 830343-49-2D,
base pairing with guanine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(new four-base genetic Helix, yDNA, composed of widened
benzopyrimidine-purine pairs)
RN 830343-25-4 ZCAPLUS
CN 2,4(1H,3H)-Quinazolin-2-one, 6-(2-deoxy-β-D-erythro-pentofuranosyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 830343-49-2 ZCAPLUS
CN 4(1H)-Quinazolin-2-one, 2-amino-6-(2-deoxy-β-D-erythro-pentofuranosyl)-8-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 850162-05-9 850162-15-1 850162-27-5
850162-30-0 850162-32-2 850162-35-5
850162-37-7 850162-39-9 850162-43-5
850162-45-7 850162-48-0 850163-10-9

850163-14-3

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)(new four-base genetic Helix, yDNA, composed of widened
benzopyrimidine-purine pairs)

RN 850162-05-9 ZCAPLUS

CN 3'-Guanylic acid, 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-
1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-
1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-
2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-1'-(2-
amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-
yl)-2'-deoxyadenylyl-(3'→5')-2'-deoxy-, complex with
1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
purin-9-yl)-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-
(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-
de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-
dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-
deoxyguanylyl-(3'→5')-2'-deoxy-3'-guanylic acid (1:1) (9CI) (CA
INDEX NAME)

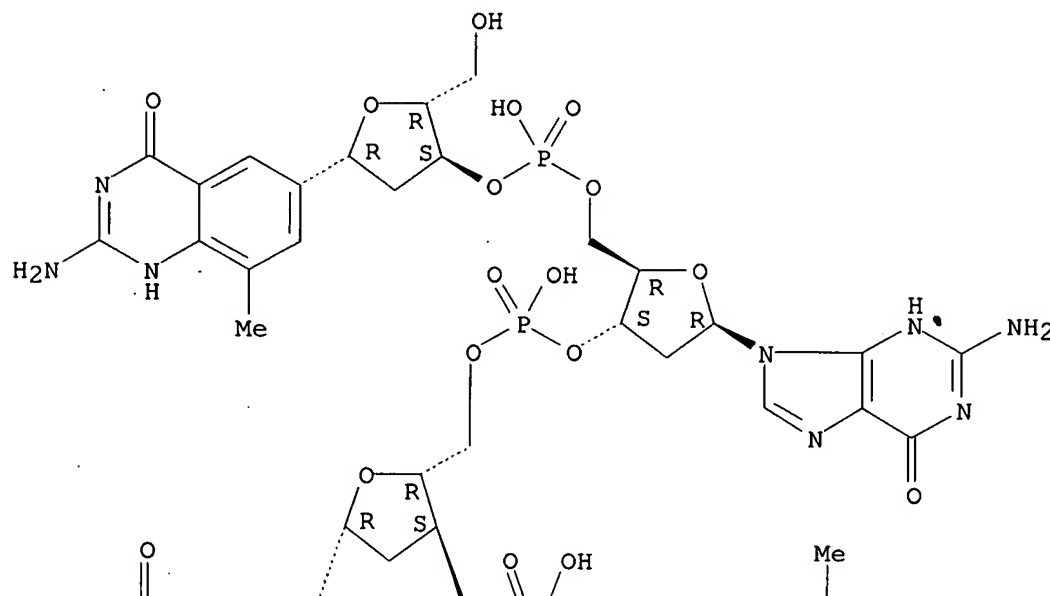
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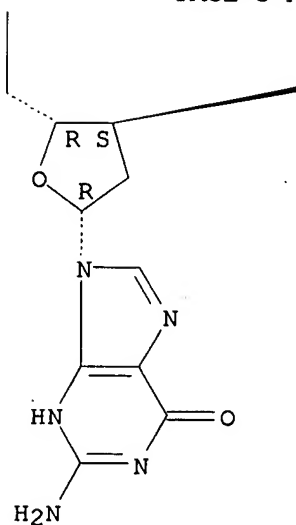
CMF C82 H98 N29 O43 P7

Absolute stereochemistry.

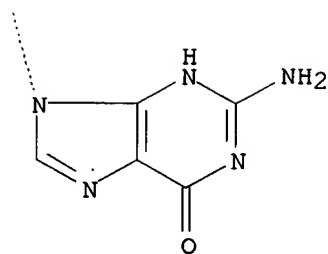
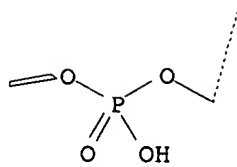
PAGE 1-A



PAGE 3-A



PAGE 3-B

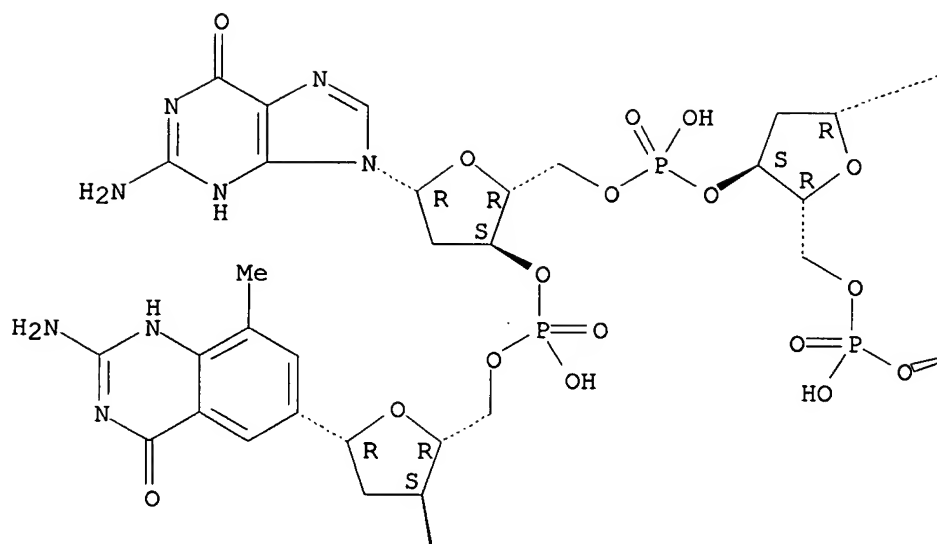


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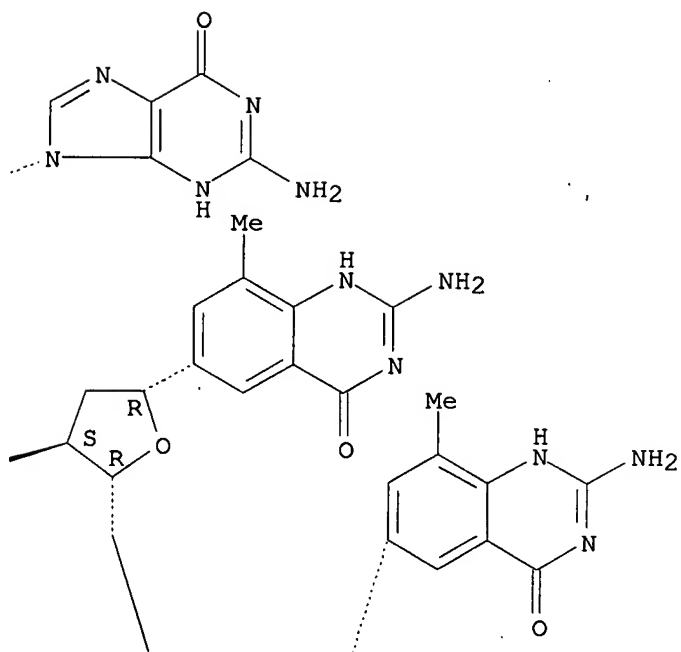
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Absolute stereochemistry.

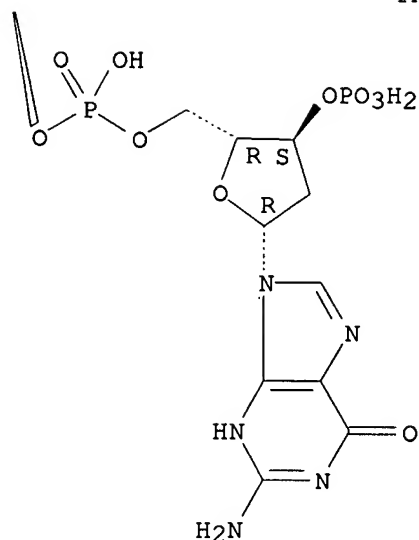
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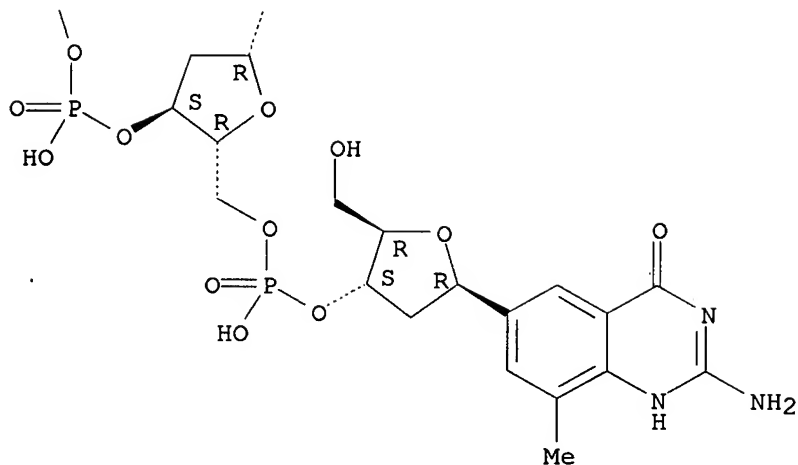
PAGE 1-B



PAGE 2-A



PAGE 2-B



RN 850162-15-1 ZCAPLUS
 CN 3'-Guanylic acid, 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-
 1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-
 (1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-2'-
 deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-2'-deoxy-, complex with 1'-(2-amino-1,4-
 dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-2'-deoxy-3'-guanylic acid (1:1) (9CI) (CA INDEX NAME)

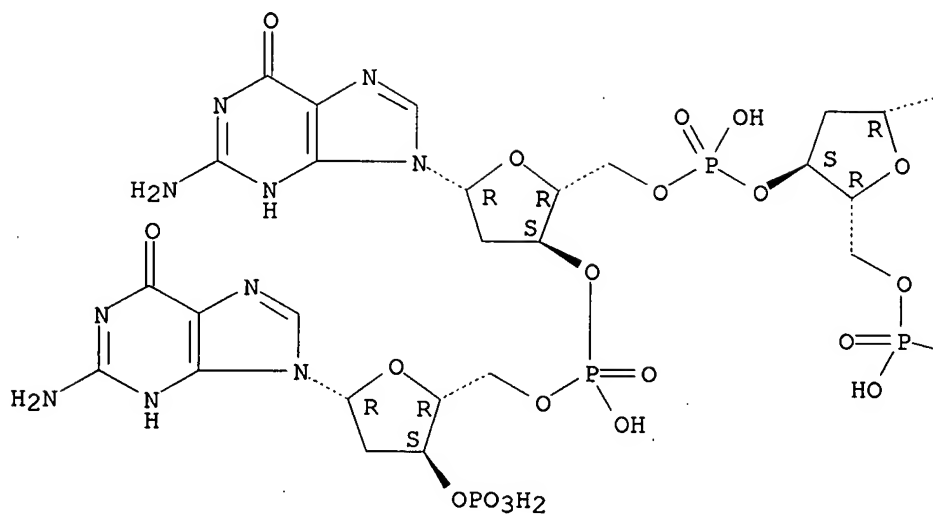
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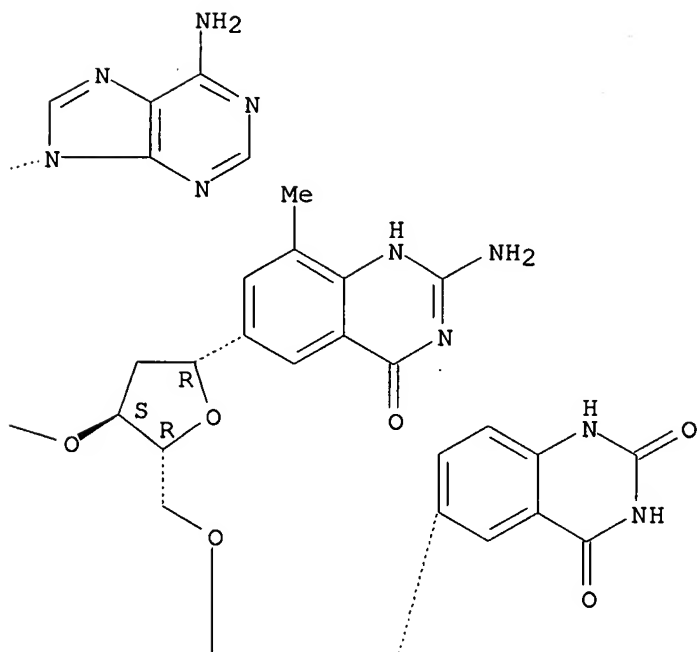
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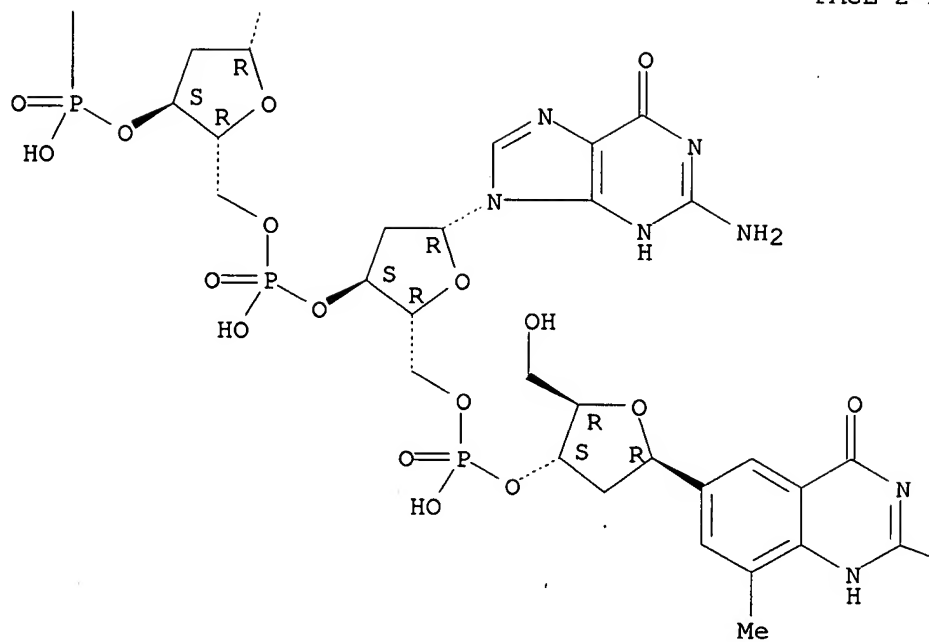
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





NH₂

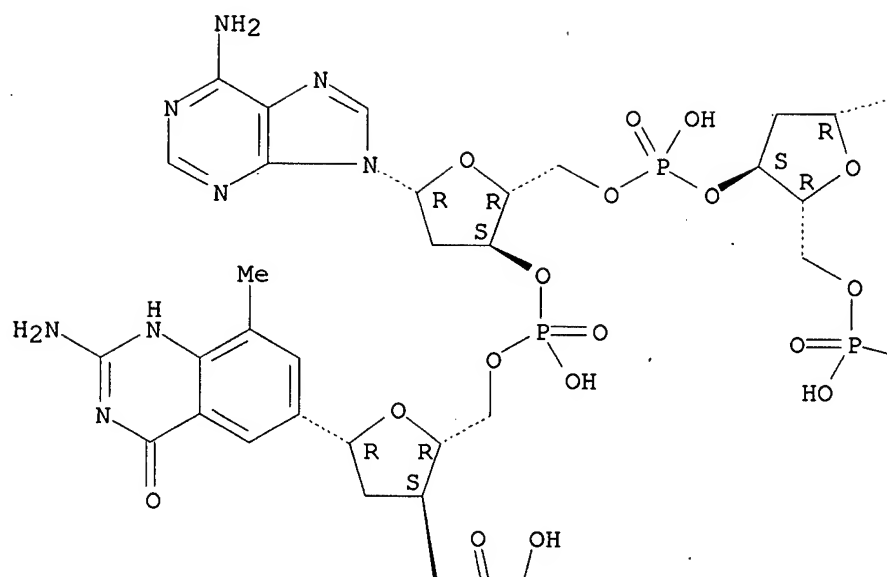
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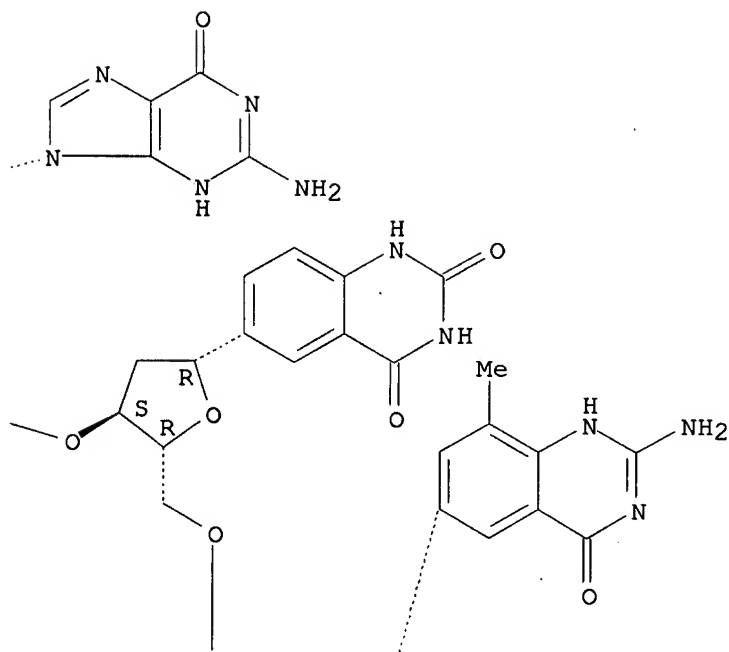
CMF C85 H99 N26 O43 P7

Absolute stereochemistry.

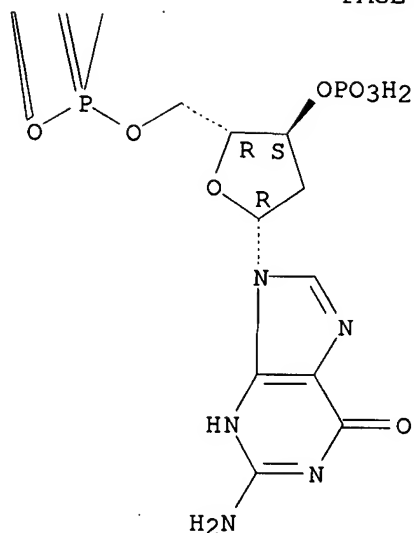
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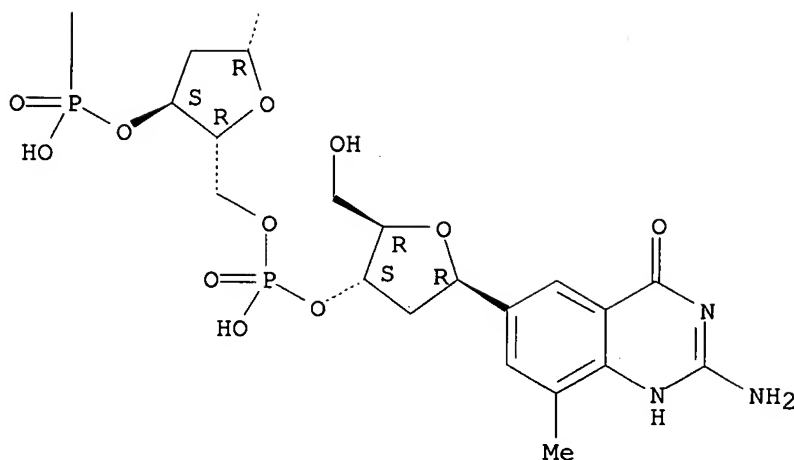
PAGE 1-B



PAGE 2-A



PAGE 2-B



RN 850162-27-5 ZCAPLUS

CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1)

10/ 530,897

(9CI) (CA INDEX NAME)

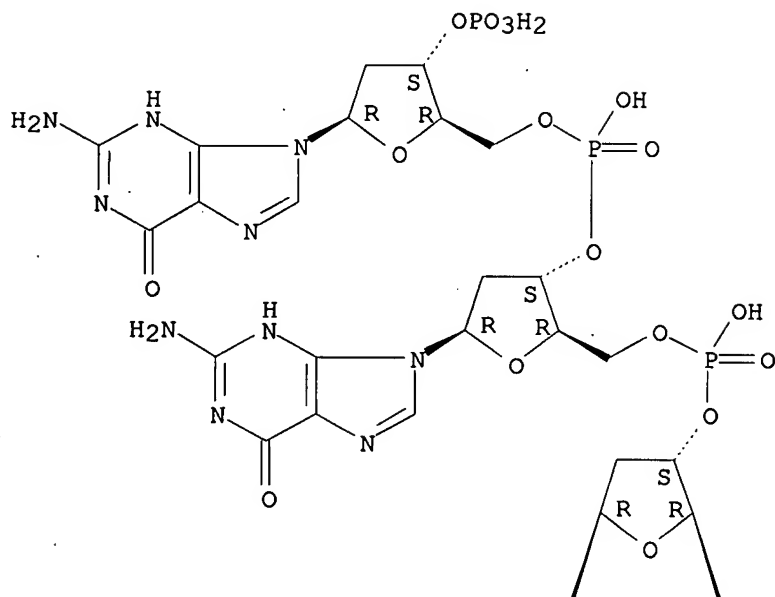
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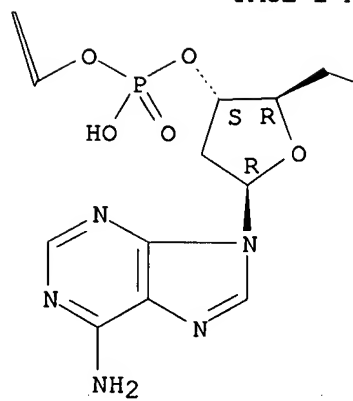
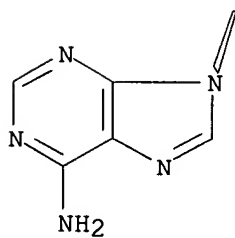
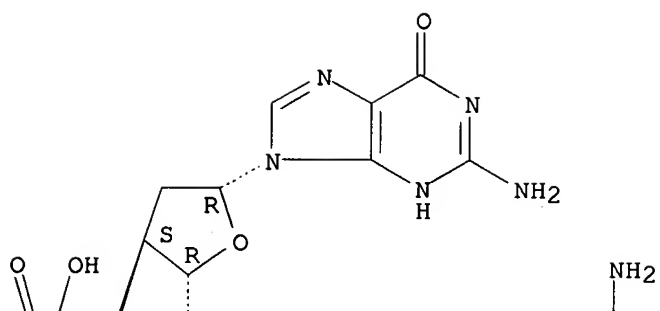
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CMF C80 H98 N40 O46 P8

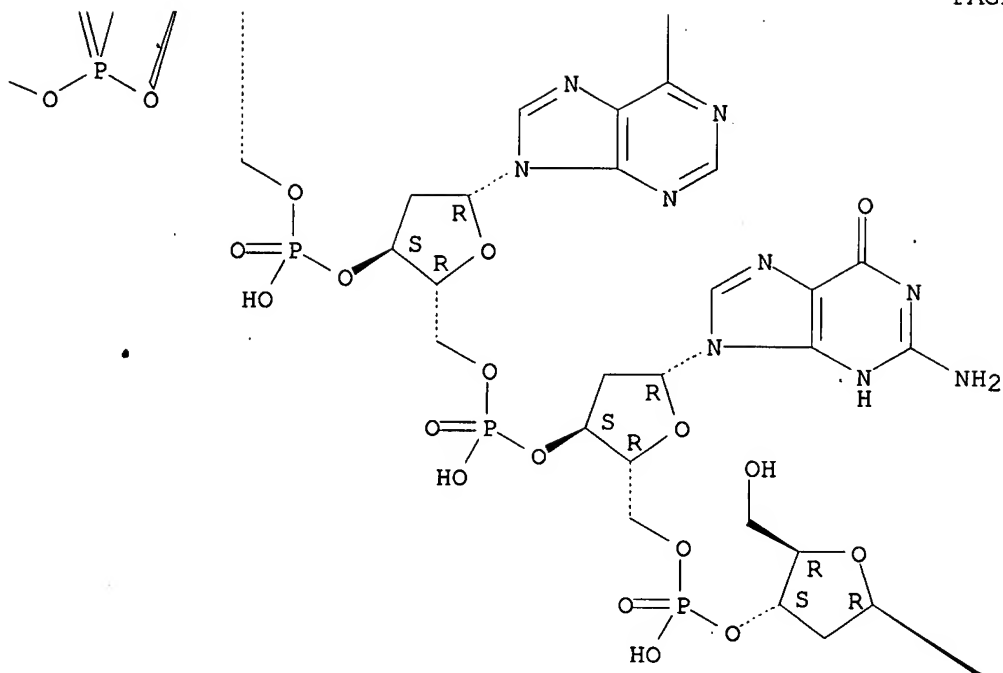
Absolute stereochemistry.

PAGE 1-A



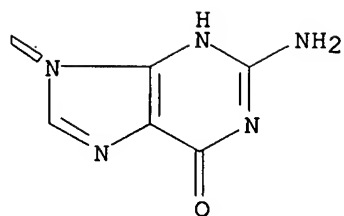


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PAGE 3-B

PAGE 3-C

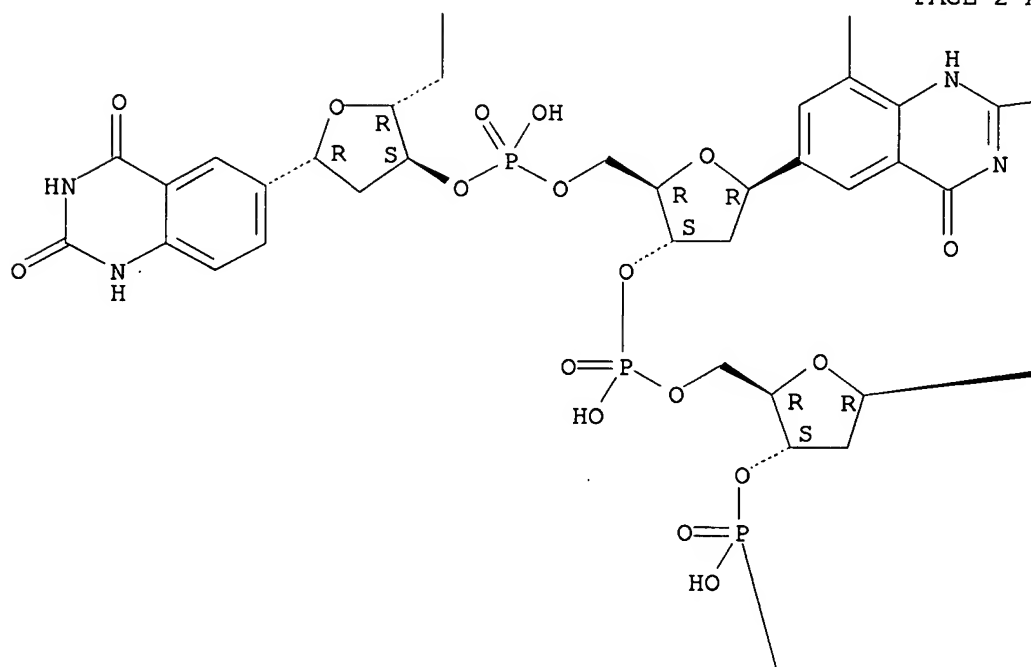
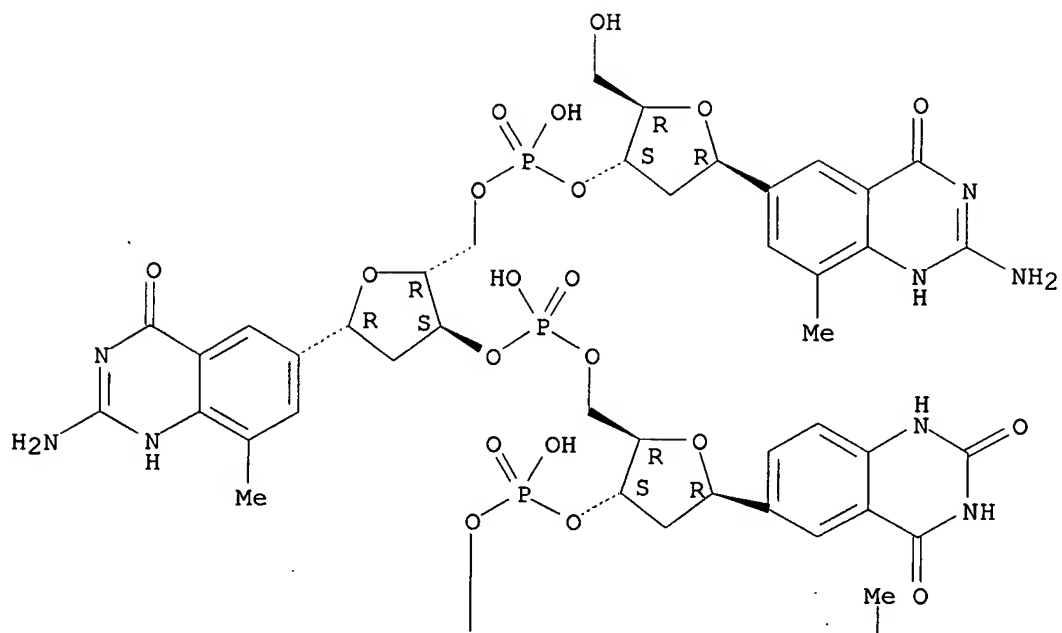


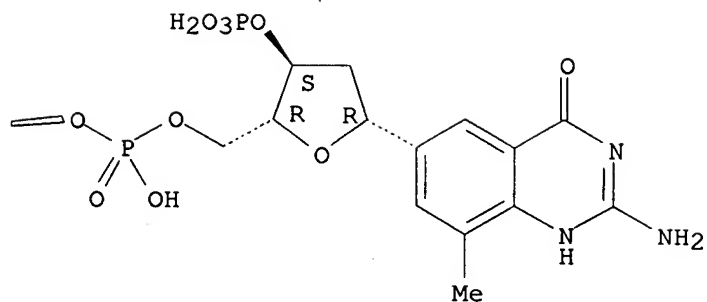
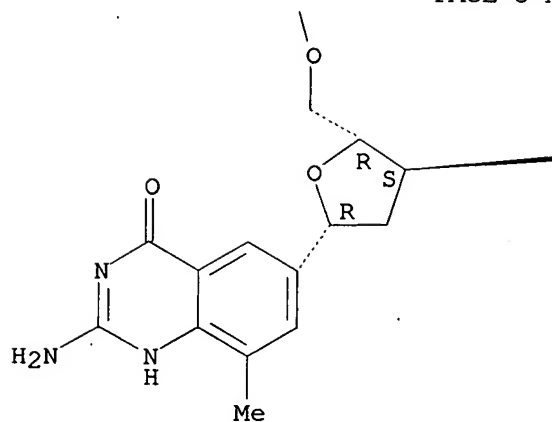
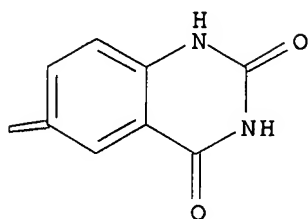
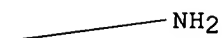
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-30-0 ZCAPLUS

CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-
(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-
(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyadenylyl-

(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
 purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-
 methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
 quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1)
 (9CI) (CA INDEX NAME)

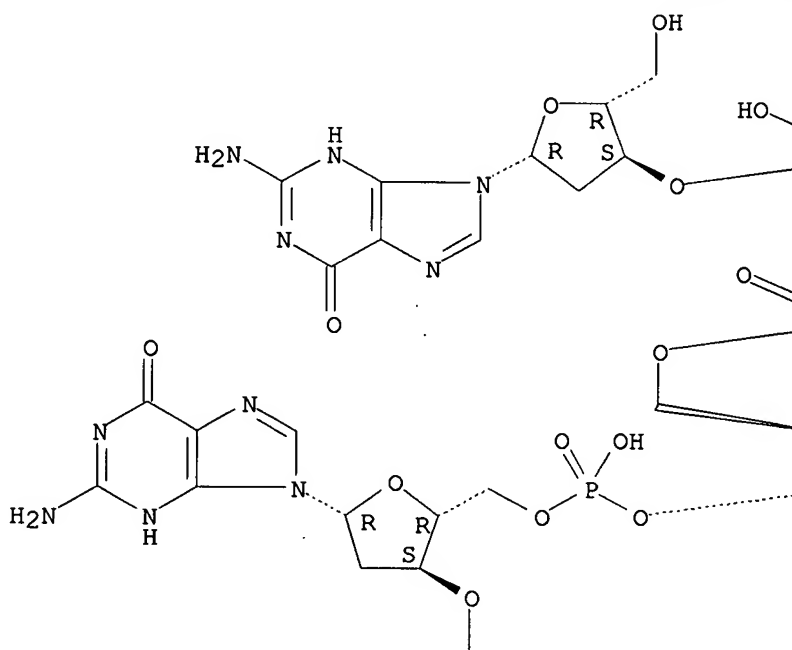
CM 1

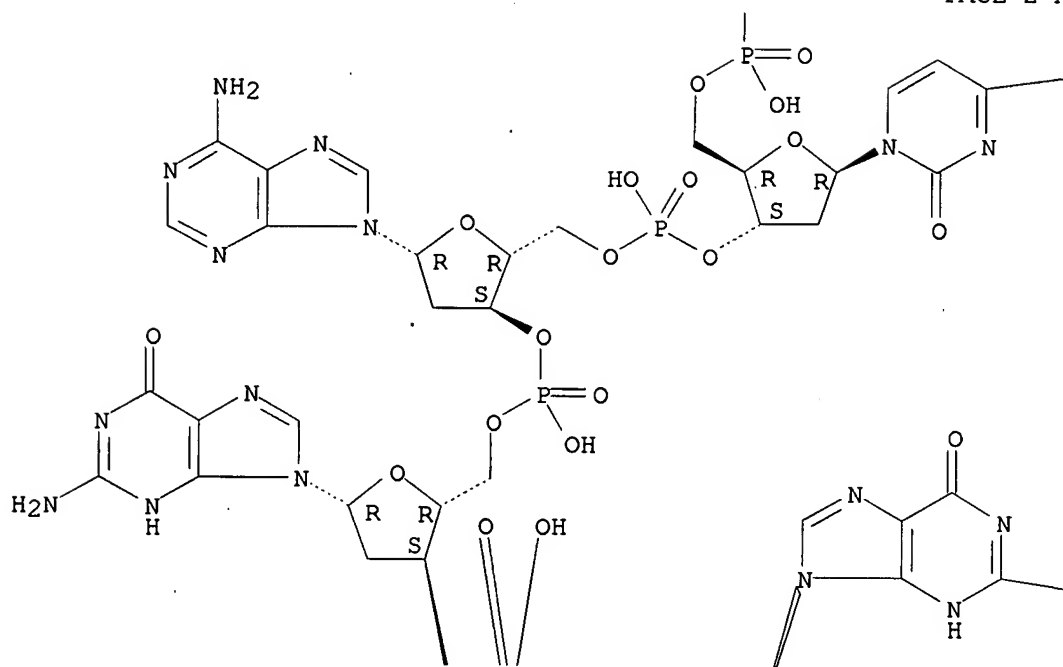
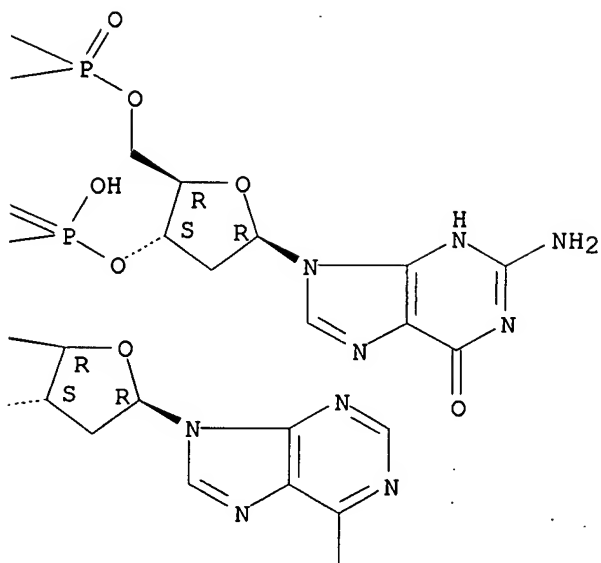
CRN 850162-29-7

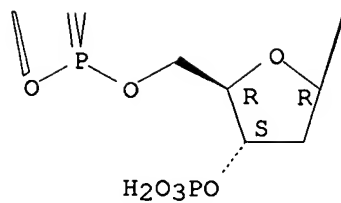
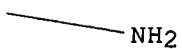
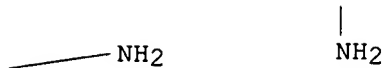
CMF C79 H98 N38 O47 P8

Absolute stereochemistry.

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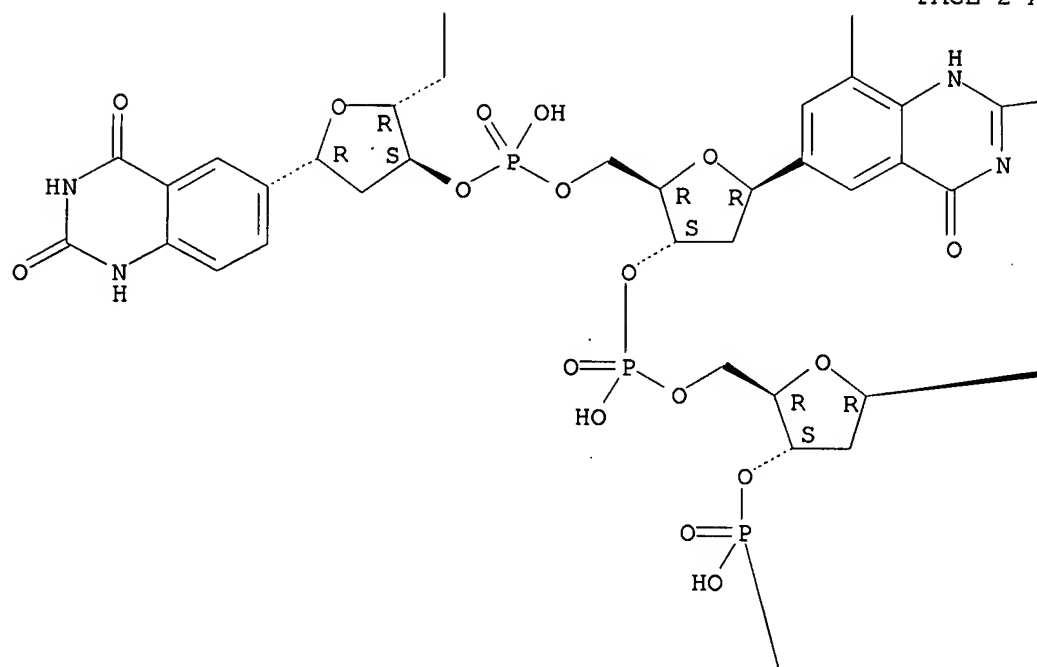
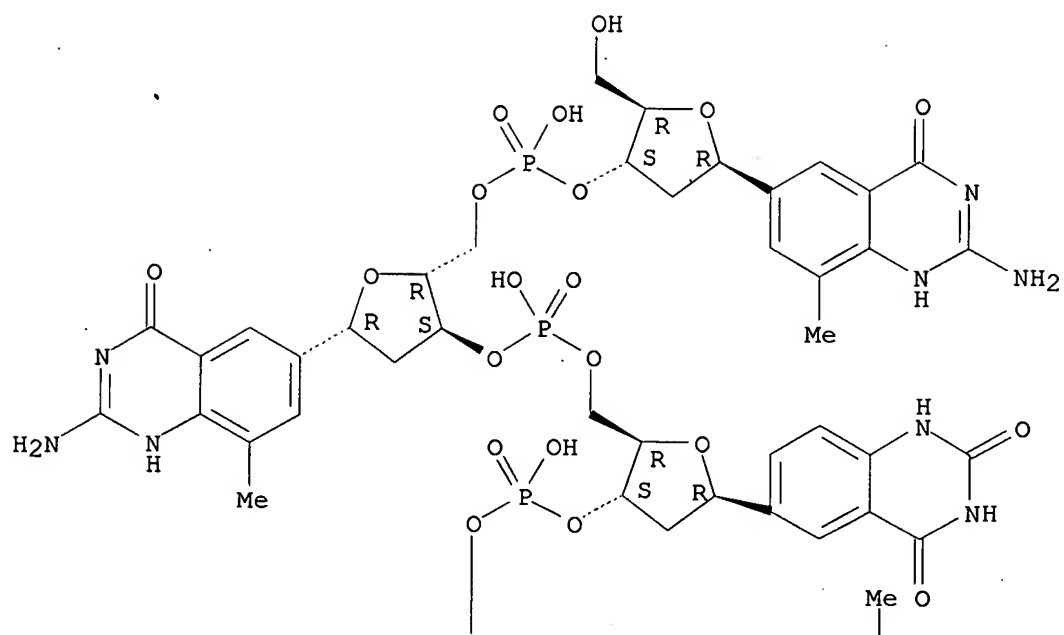


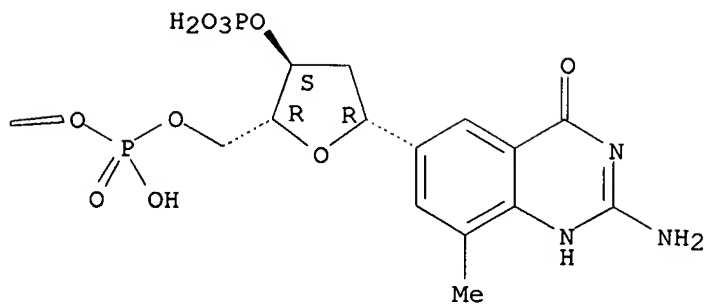
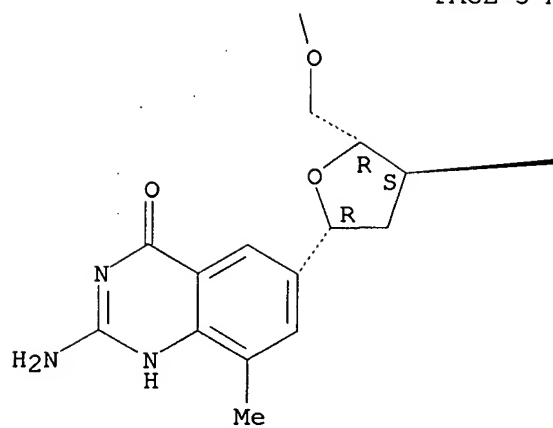
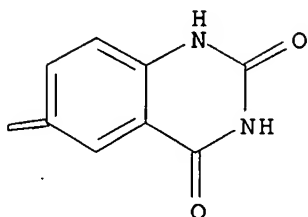
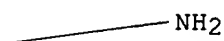
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-32-2 ZCAPLUS
 CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-

(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
 purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-
 methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
 quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1)
 (9CI) (CA INDEX NAME)

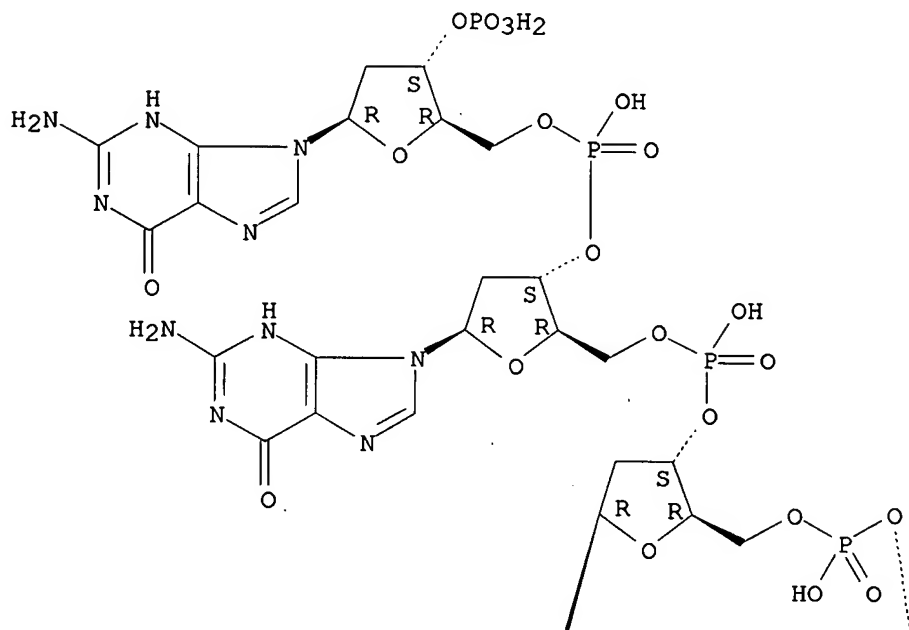
CM 1

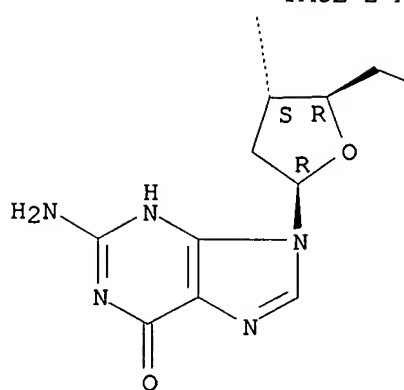
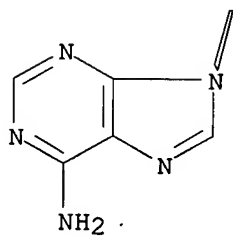
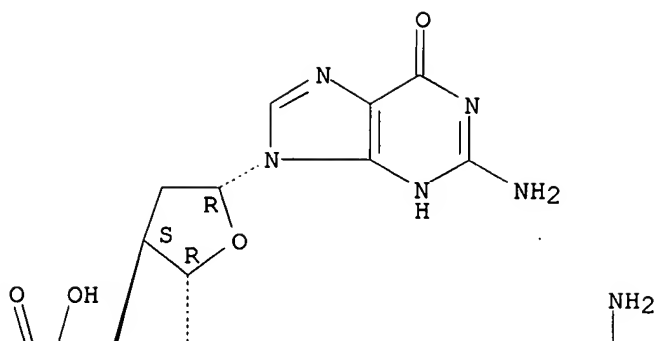
CRN 850162-31-1

CMF C80 H98 N40 O47 P8

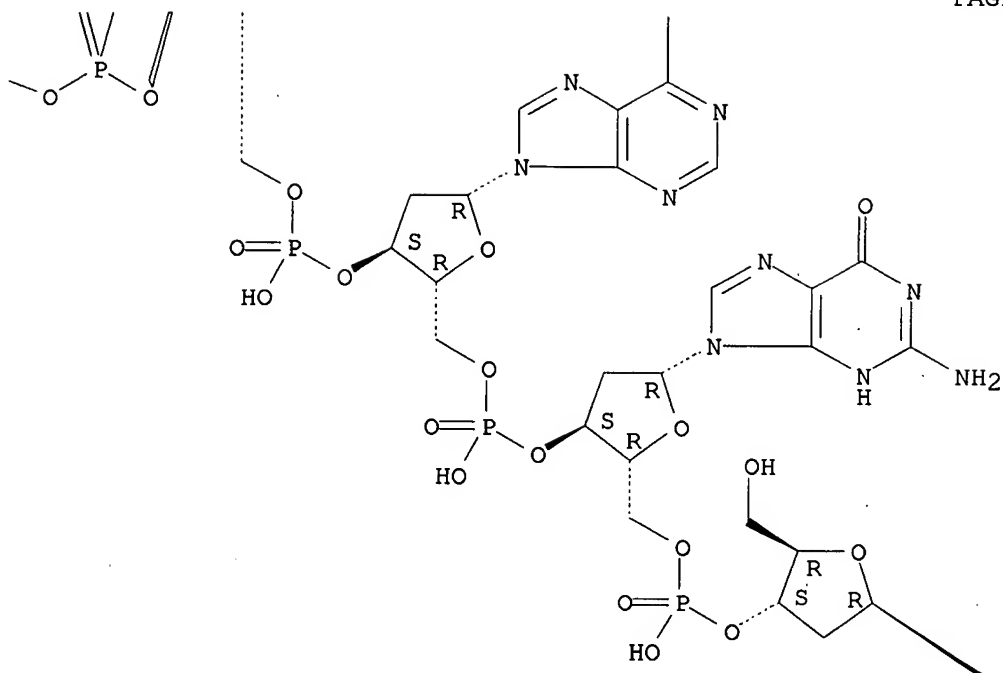
Absolute stereochemistry.

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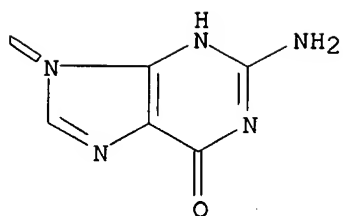


PAGE 2-B



PAGE 3-B

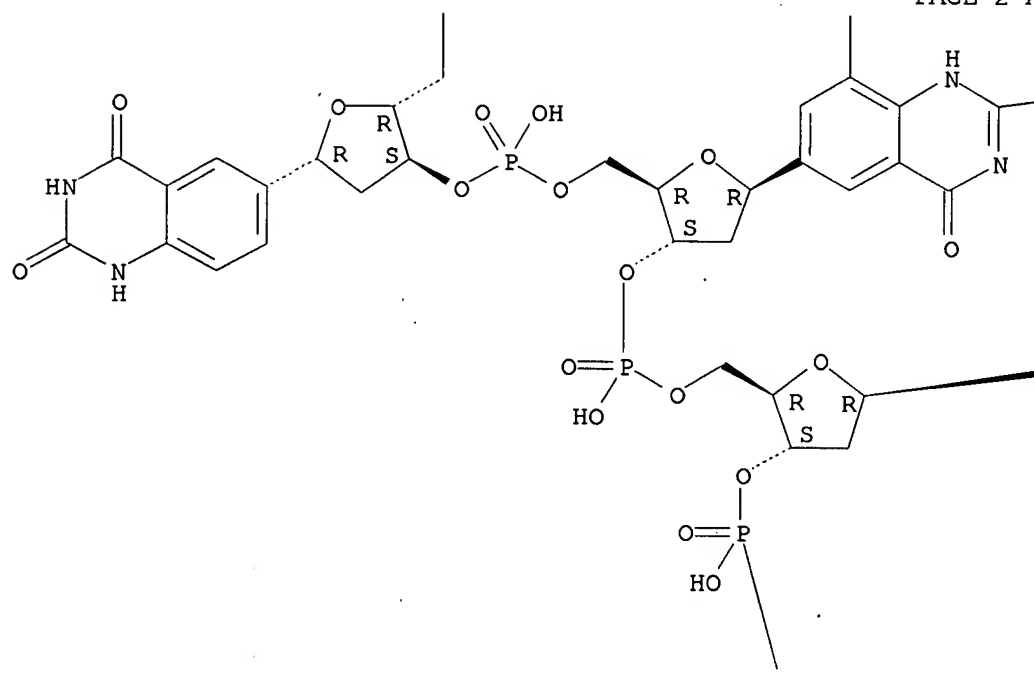
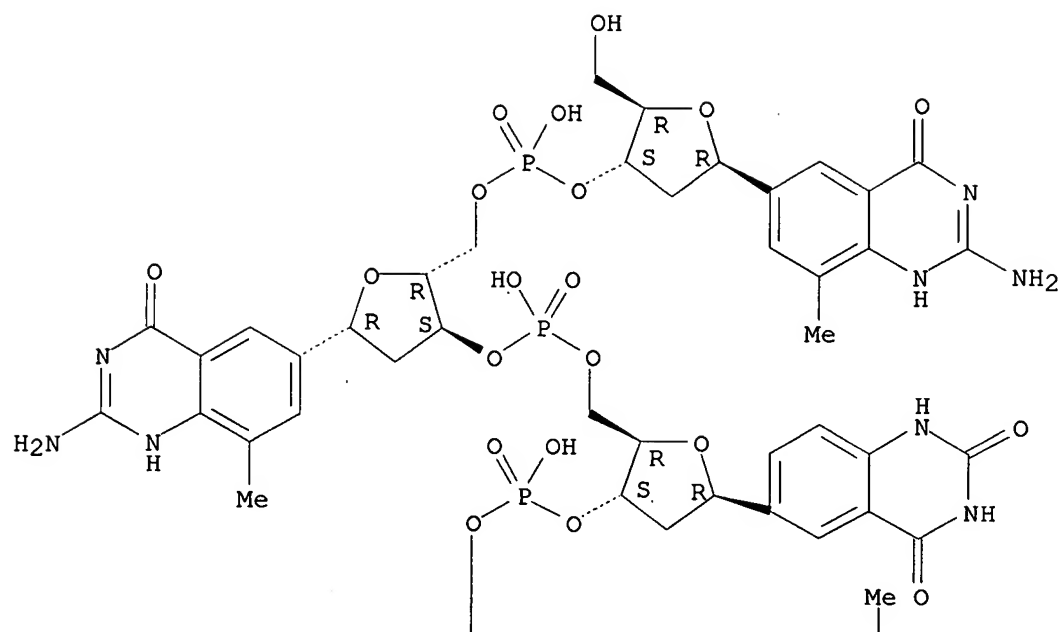
PAGE 3-C

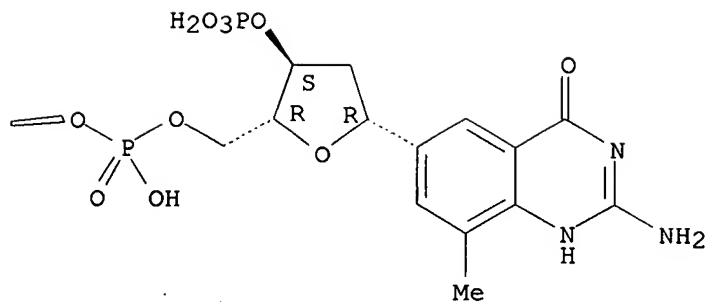
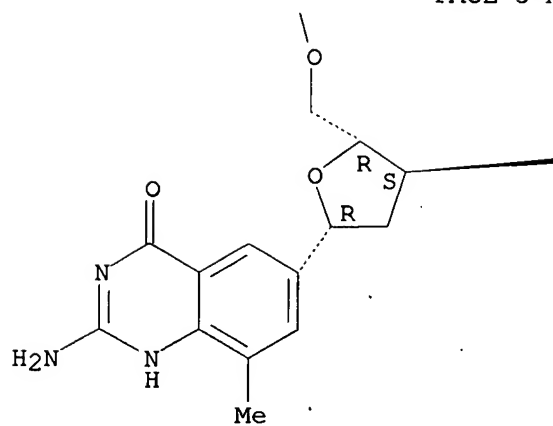
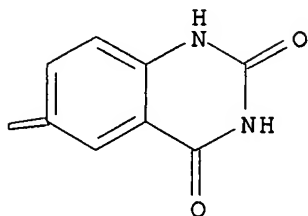
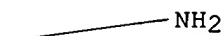


CM 2

CRN 850162-25-3
CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-35-5 ZCAPLUS
 CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-thymidylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-

2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1)
 (9CI) (CA INDEX NAME)

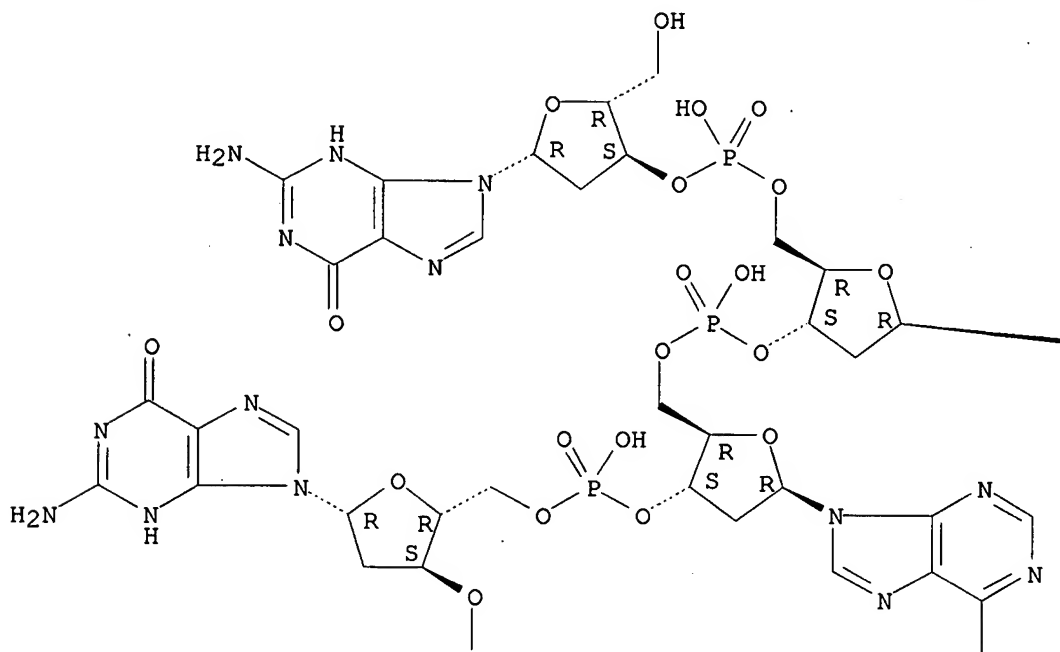
CM 1

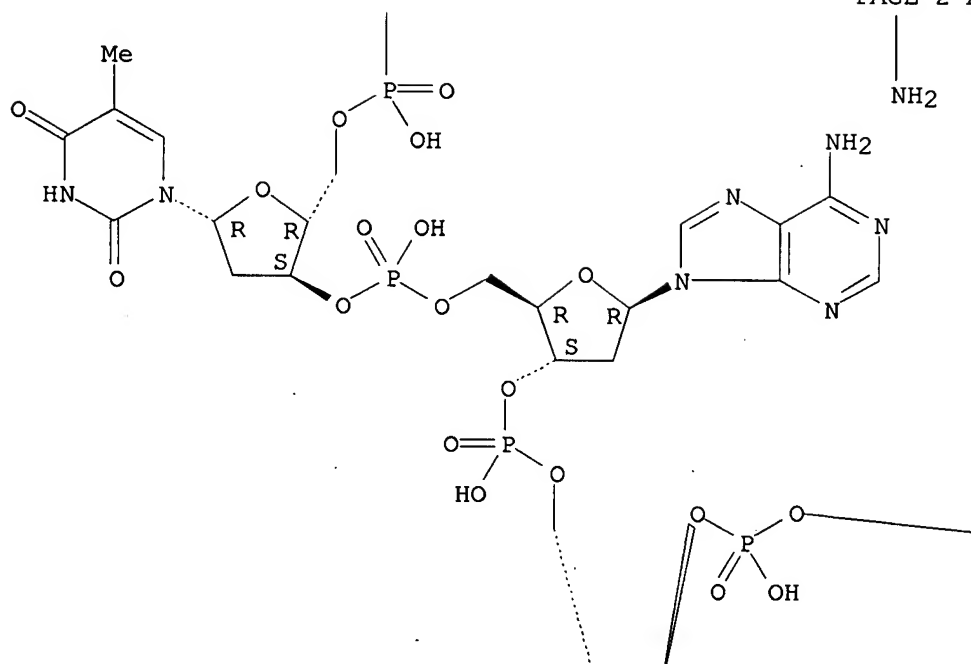
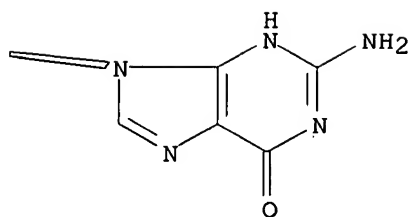
CRN 850162-34-4

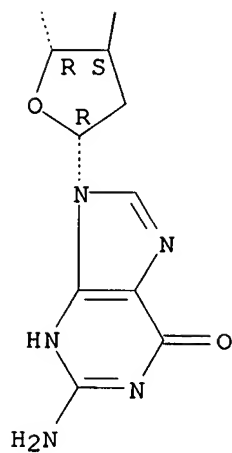
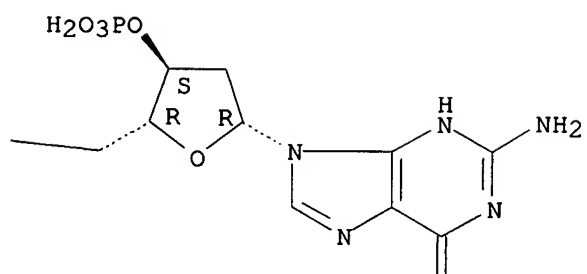
CMF C80 H99 N37 O48 P8

Absolute stereochemistry.

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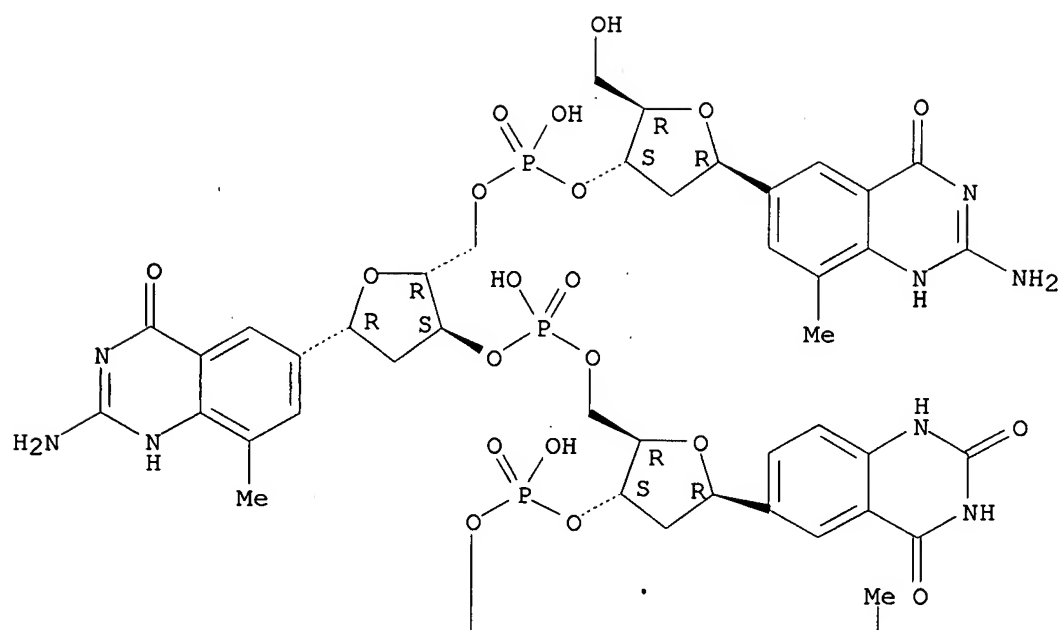




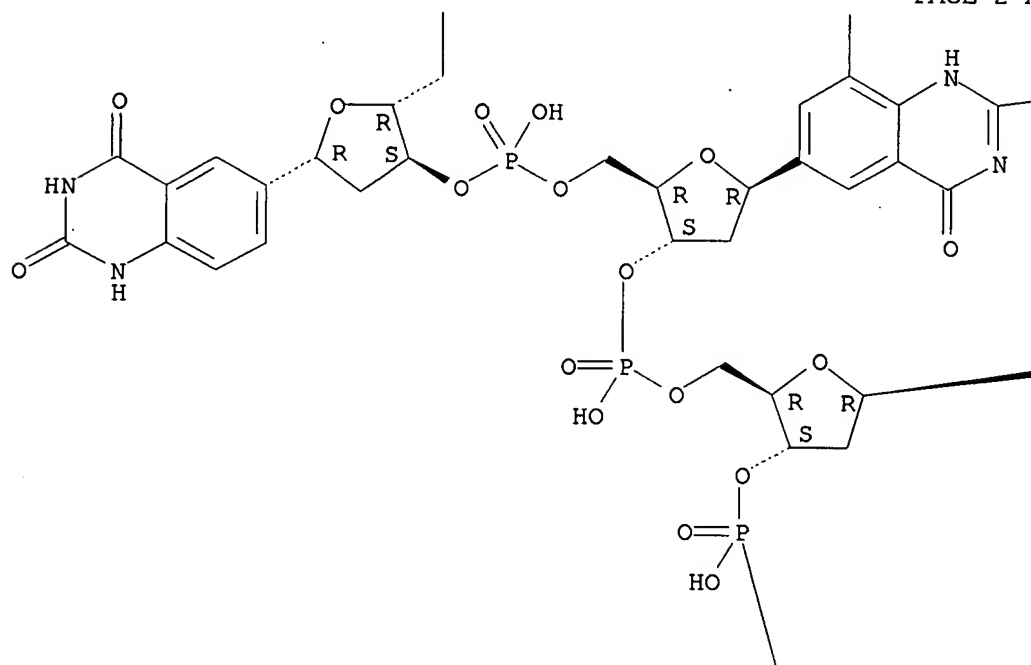
CRN 850162-25-3
CMF C109 H121 N21 O52 P8

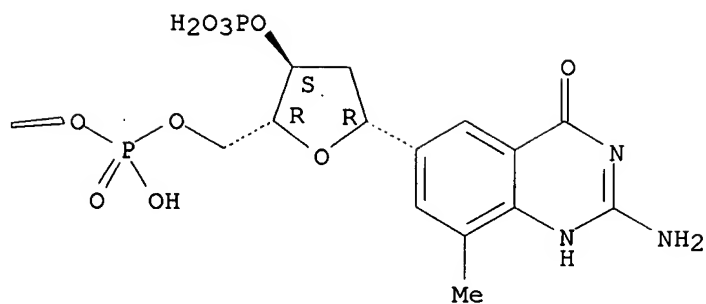
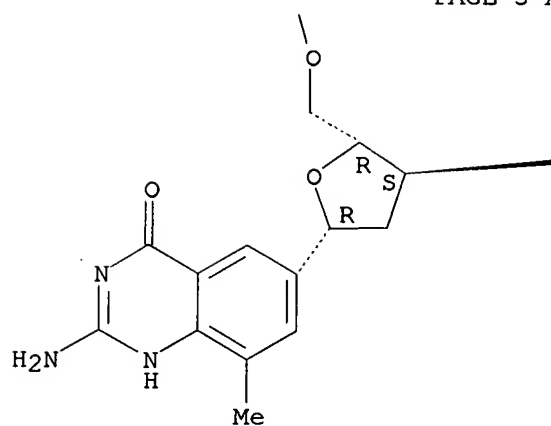
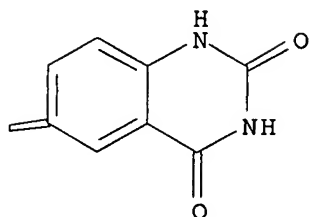
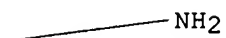
Absolute stereochemistry.

PAGE 1-A



PAGE 2-A





RN 850162-37-7 ZCAPLUS

CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-
(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-
(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-

(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
 purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-
 methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
 quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1)
 (9CI) (CA INDEX NAME)

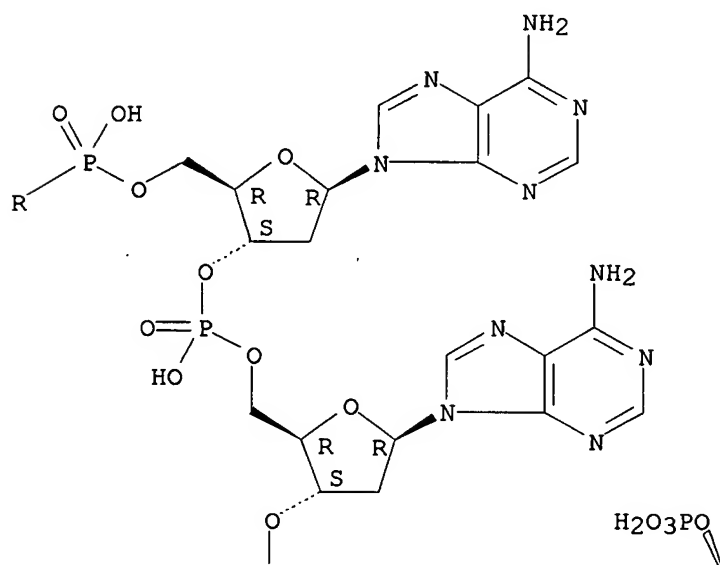
CM 1

CRN 850162-36-6

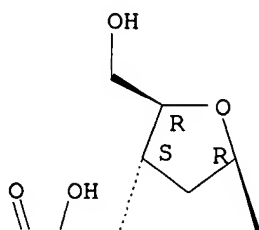
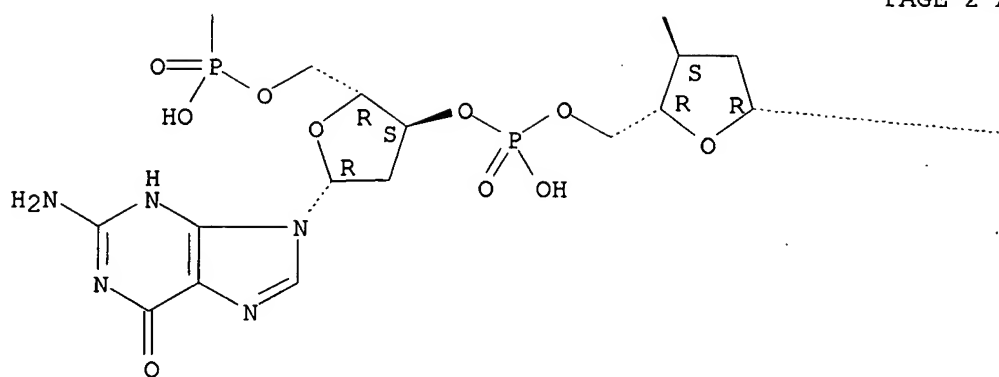
CMF C80 H98 N40 O45 P8

Absolute stereochemistry.

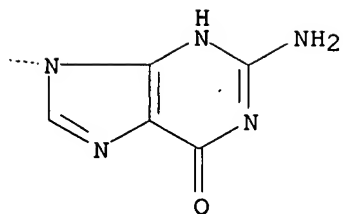
PAGE 1-A



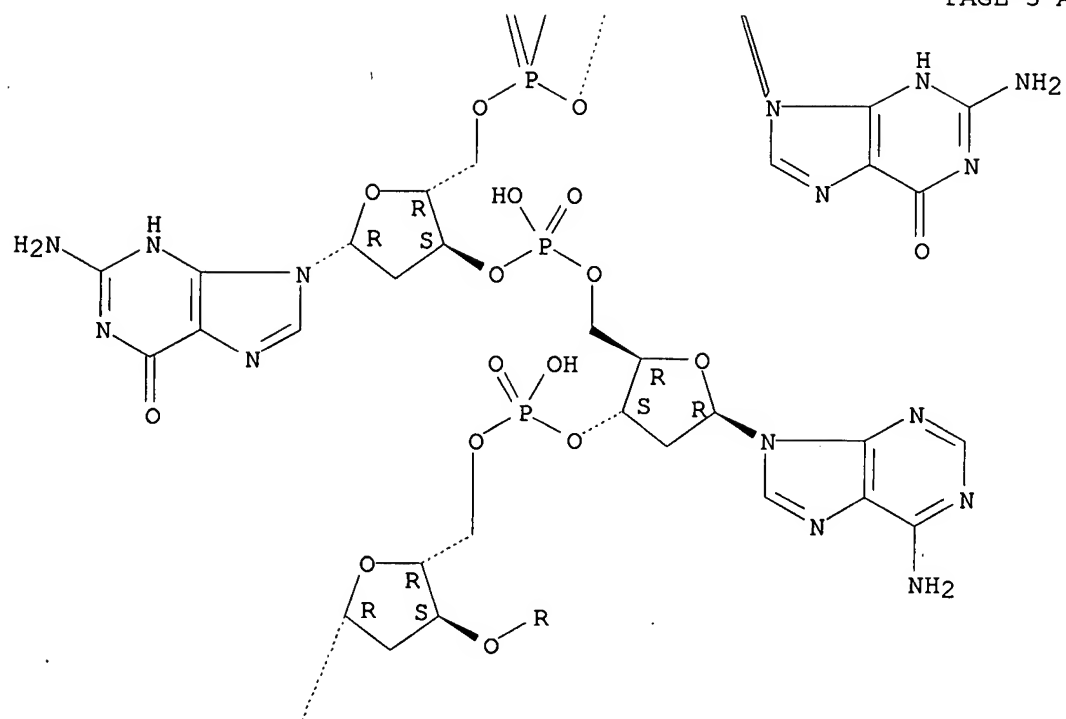
PAGE 2-A



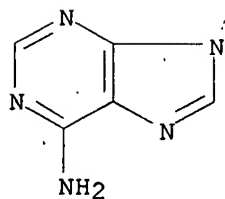
PAGE 2-B



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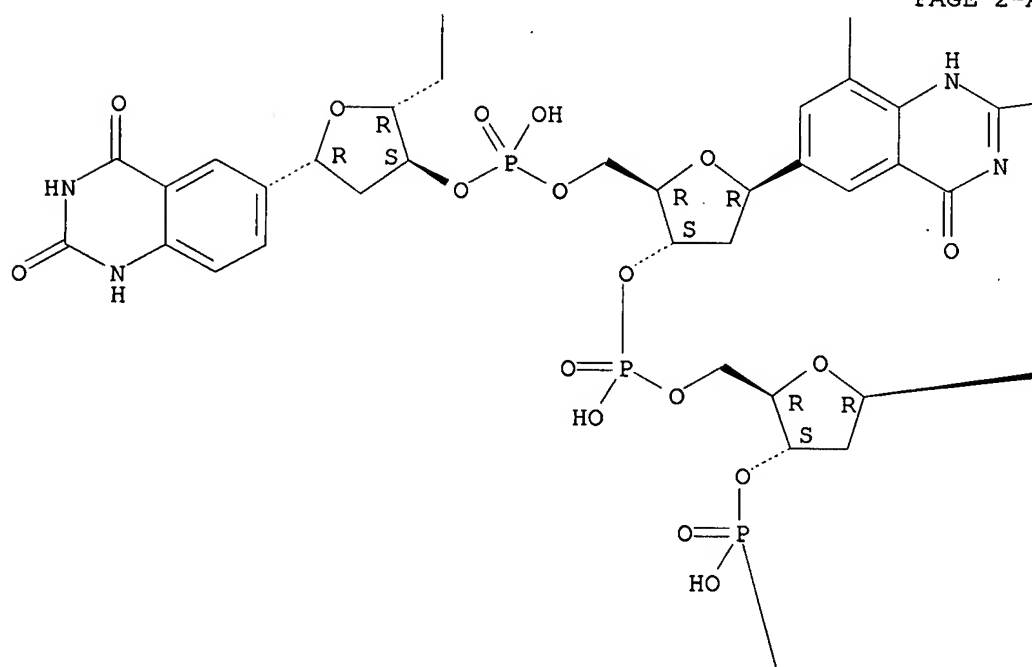
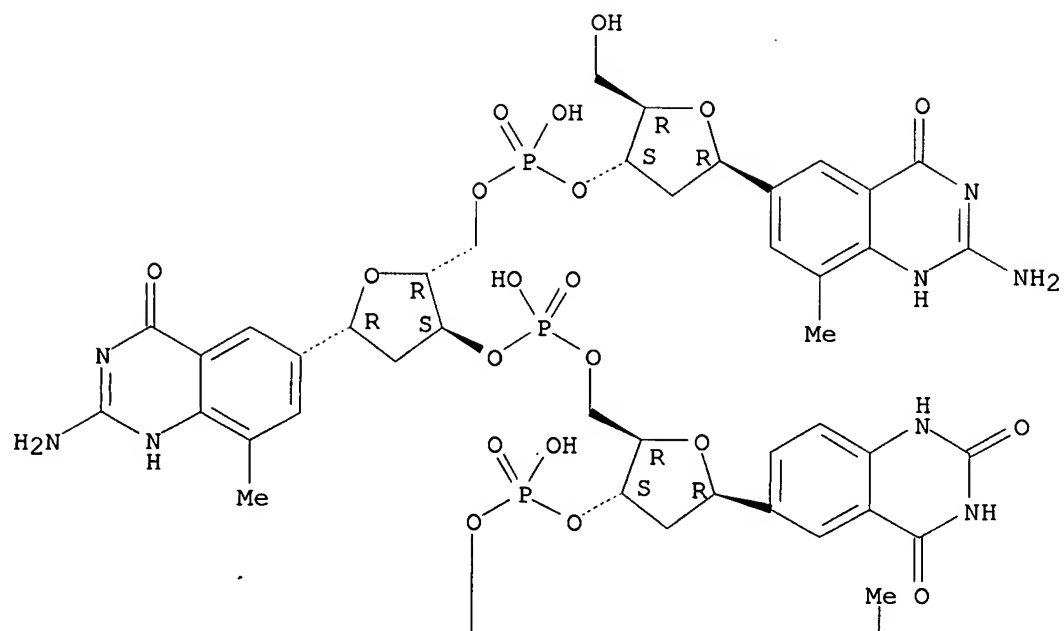


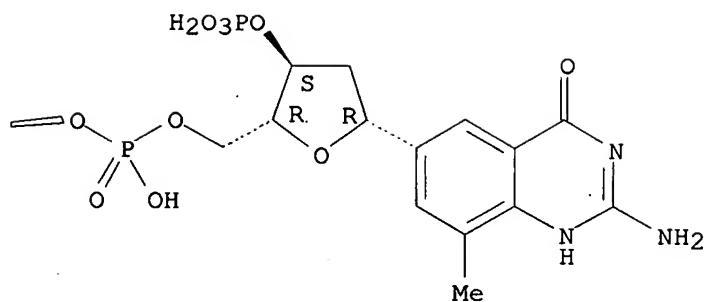
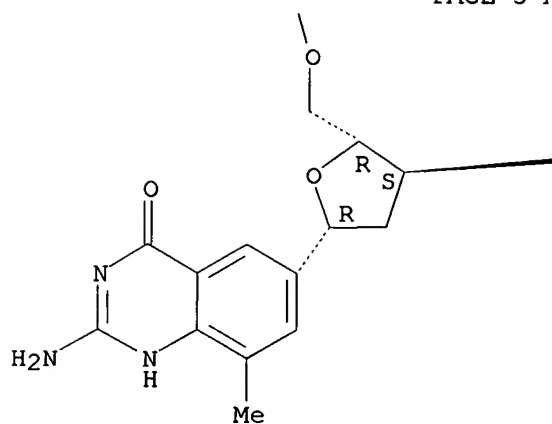
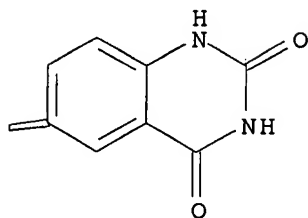
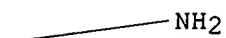
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-39-9 ZCAPLUS

CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-
 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxycytidylyl-
 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-

(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
 purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-
 methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
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 (9CI) (CA INDEX NAME)

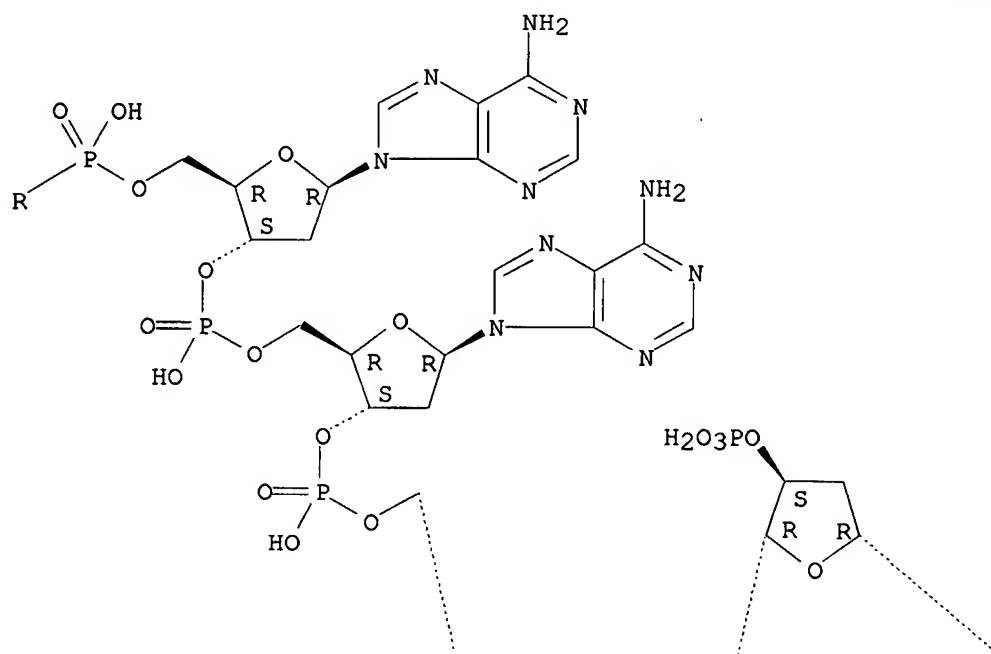
CM 1

CRN 850162-38-8

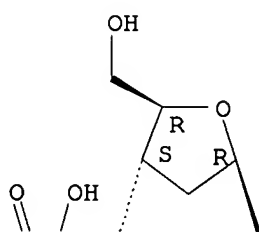
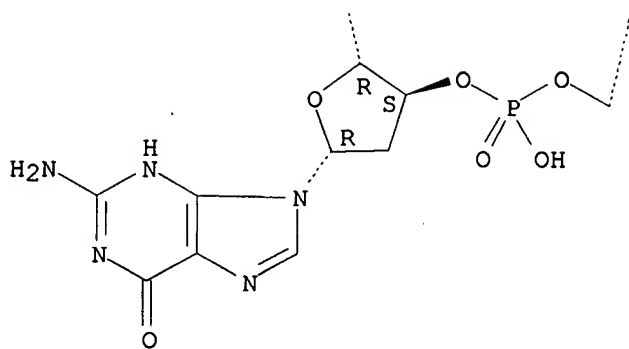
CMF C79 H98 N38 O46 P8

Absolute stereochemistry.

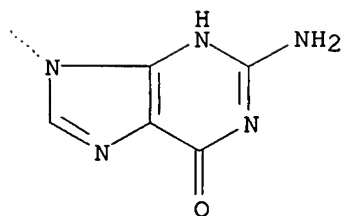
PAGE 1-A



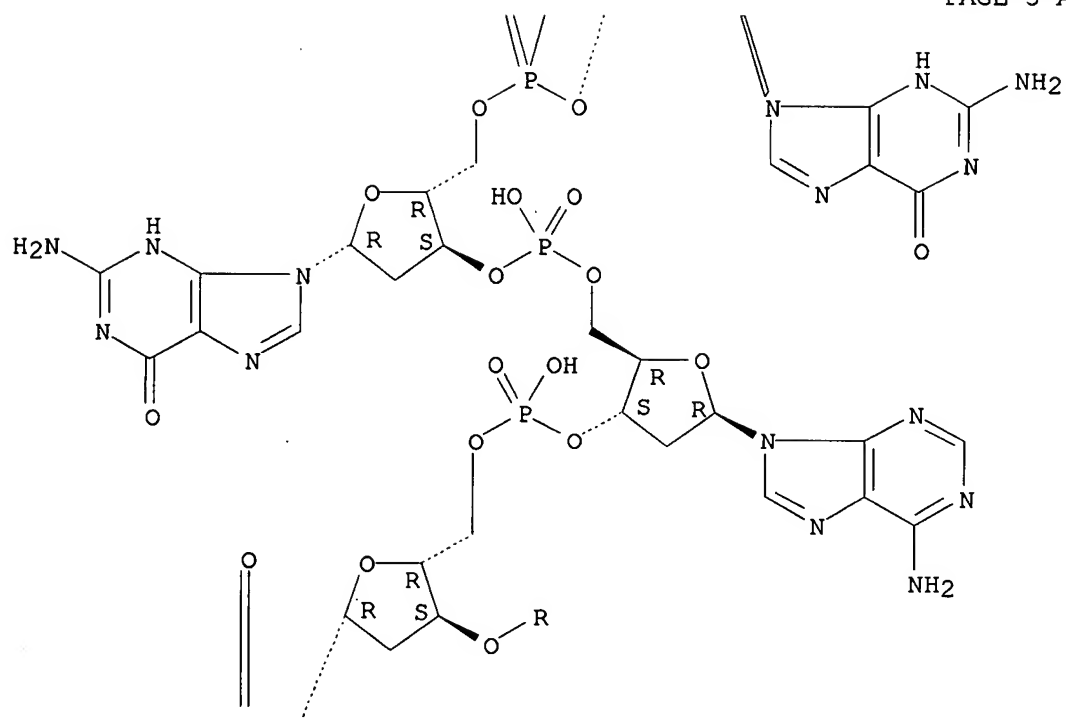
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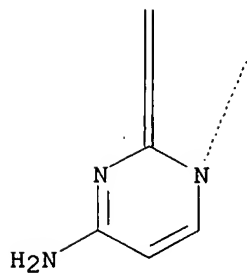
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PAGE 3-A



PAGE 4-A

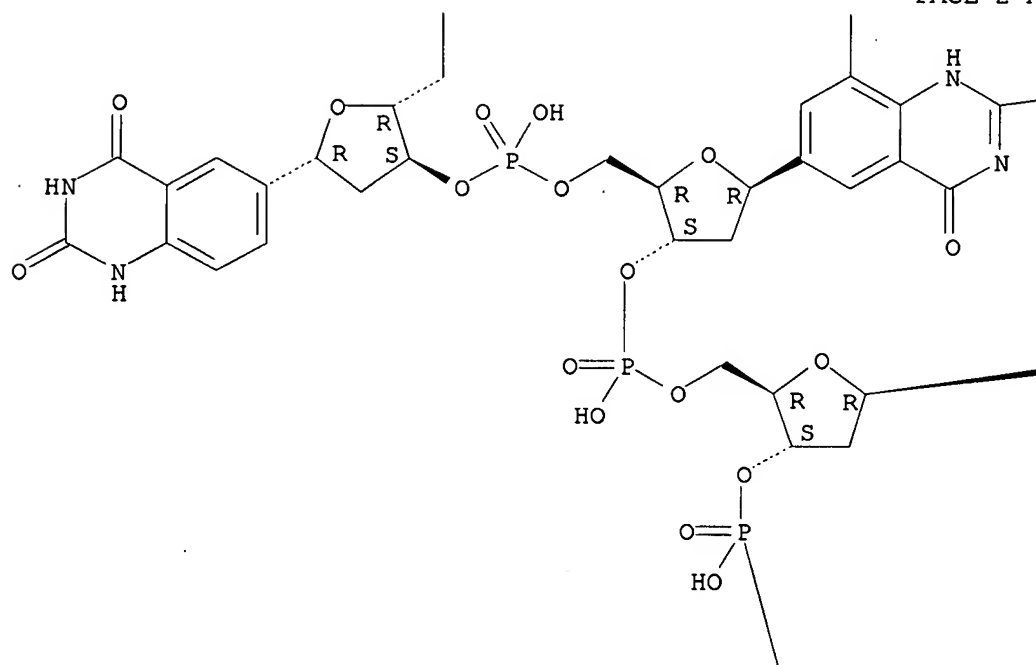
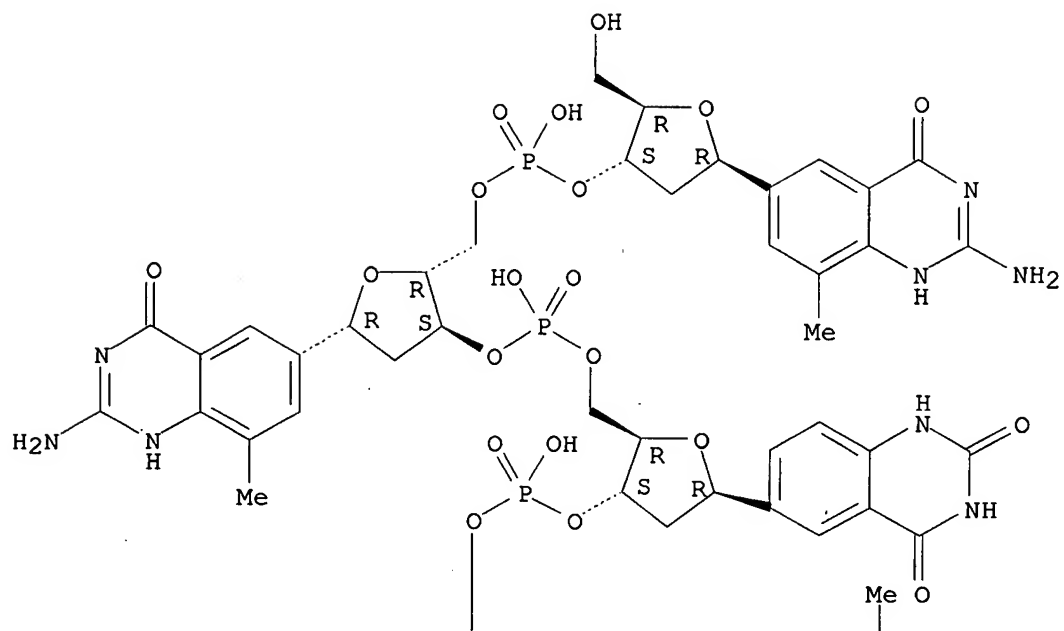


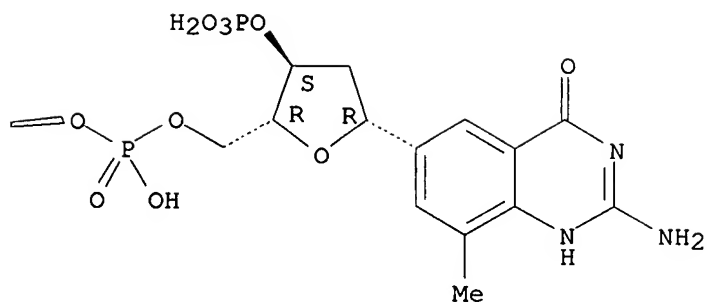
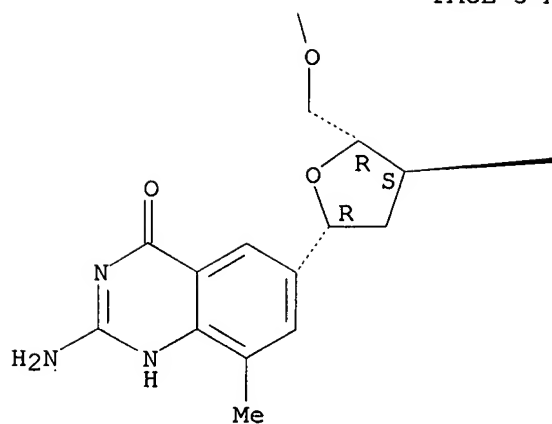
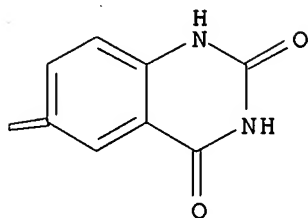
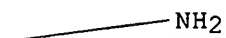
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-43-5 ZCAPLUS

CN 3'-Guanylic acid, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-thymidylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-

deoxyguanylyl-(3'→5')-2'-deoxy-, complex with 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-3'-adenylic acid (1:1) (9CI) (CA INDEX NAME)

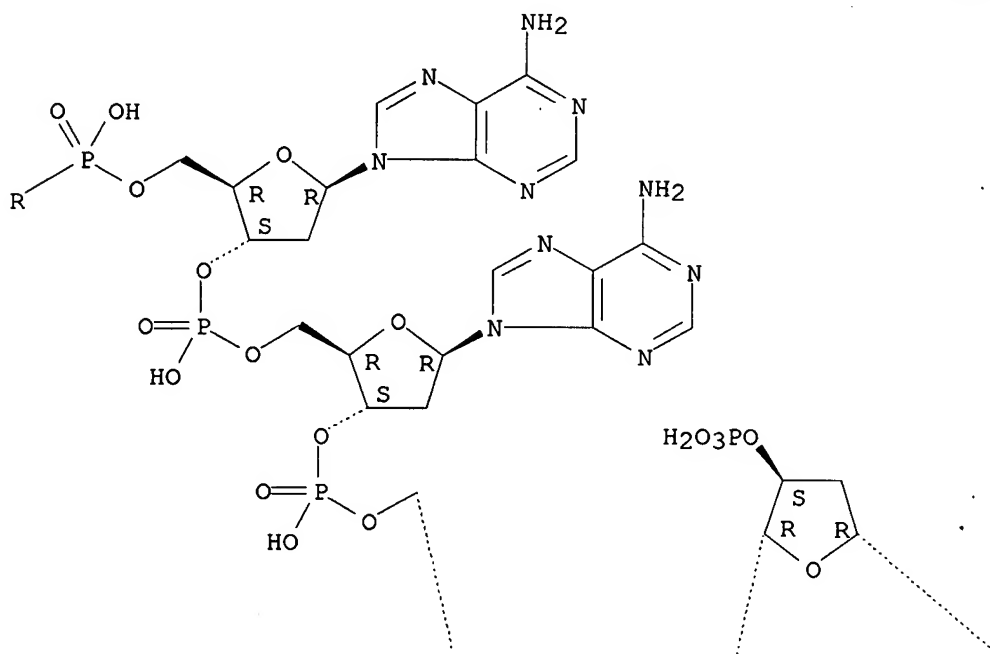
CM 1

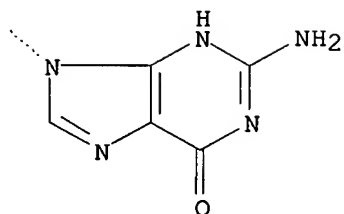
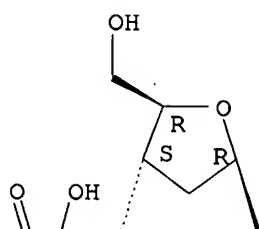
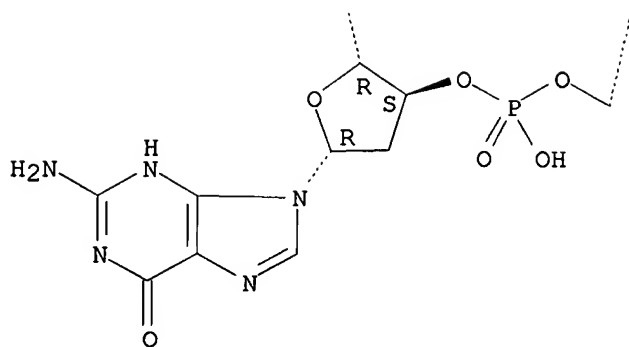
CRN 850162-42-4

CMF C80 H99 N37 O47 P8

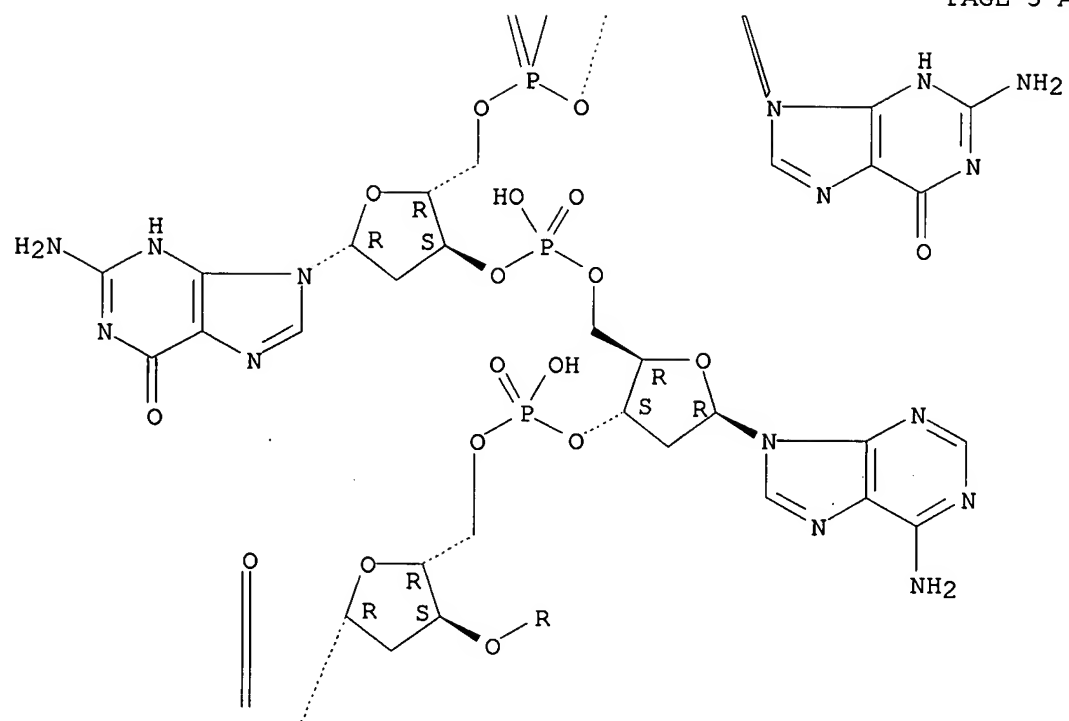
Absolute stereochemistry.

PAGE 1-A

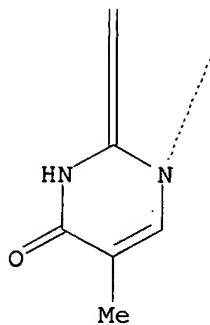




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PAGE 4-A

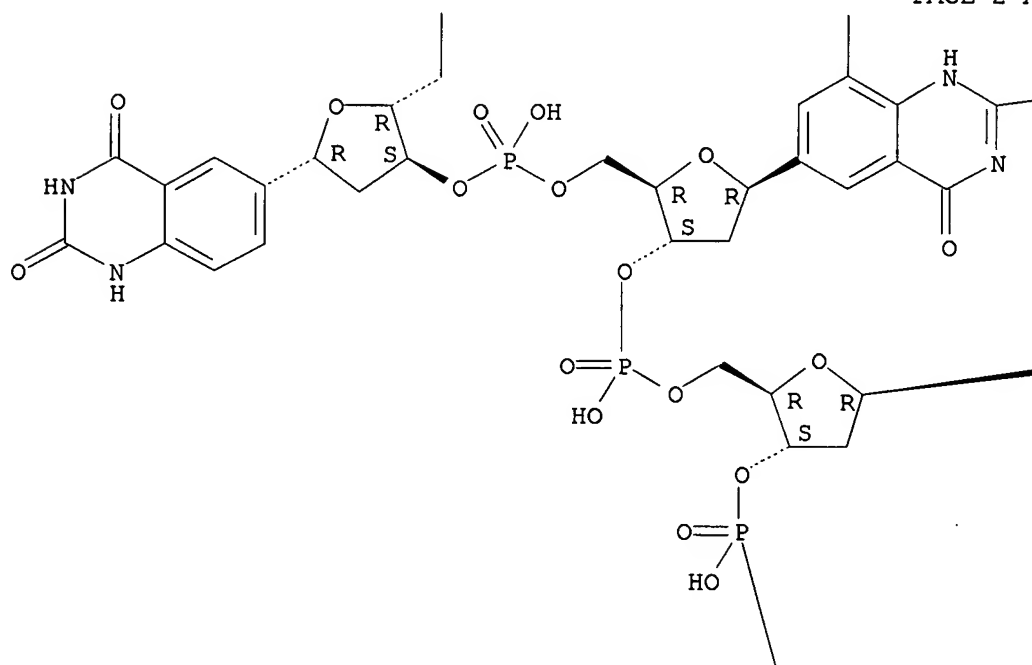
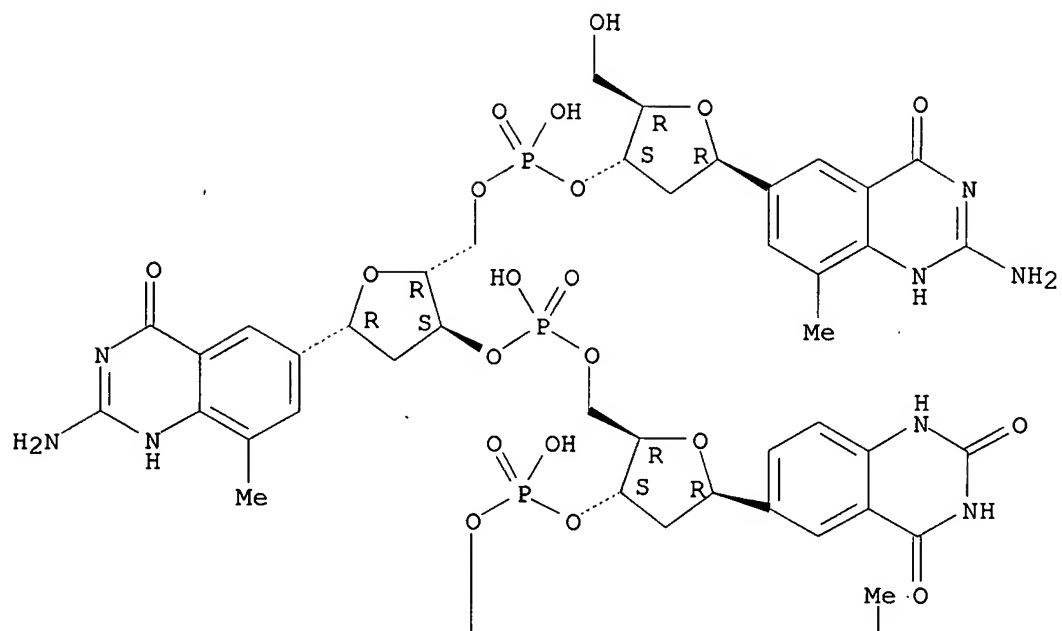


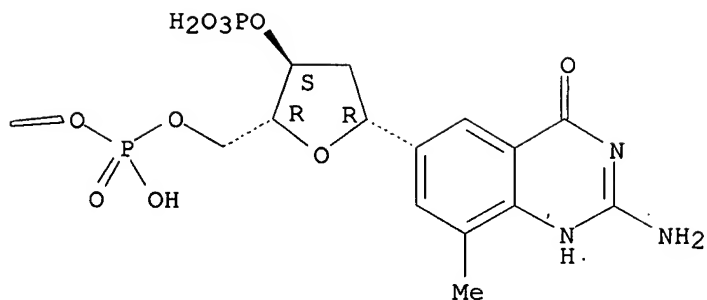
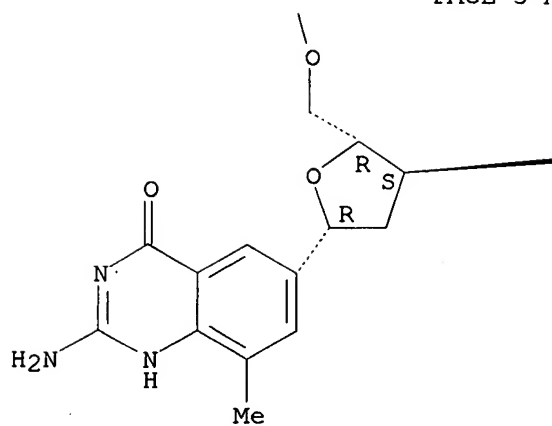
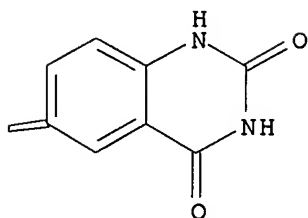
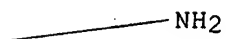
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-45-7 ZCAPLUS
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 (3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-
 (3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-

(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with
 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-
 purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-
 methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-
 9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-
 quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-
 oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-
 (3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-
 tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-
 deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
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 (9CI) (CA INDEX NAME)

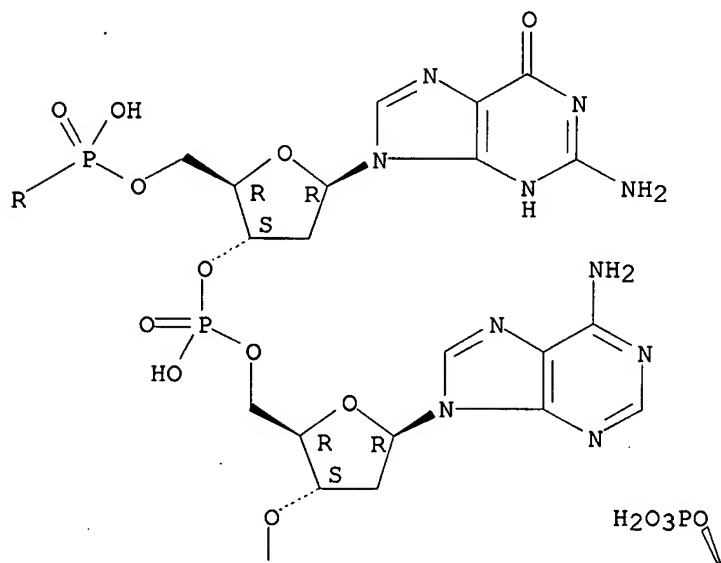
CM 1

CRN 850162-44-6

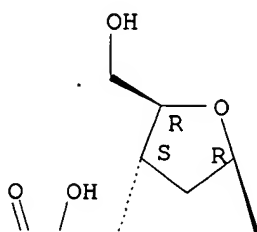
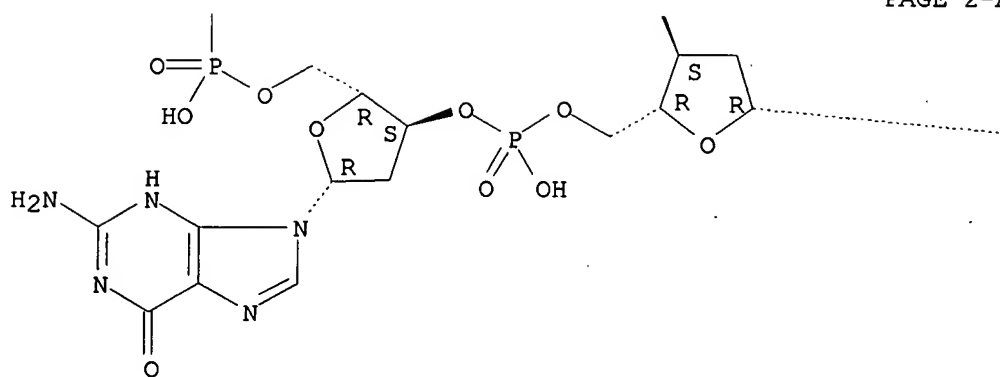
CMF C80 H98 N40 O46 P8

Absolute stereochemistry.

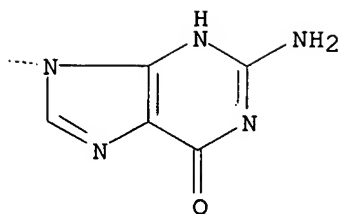
PAGE 1-A



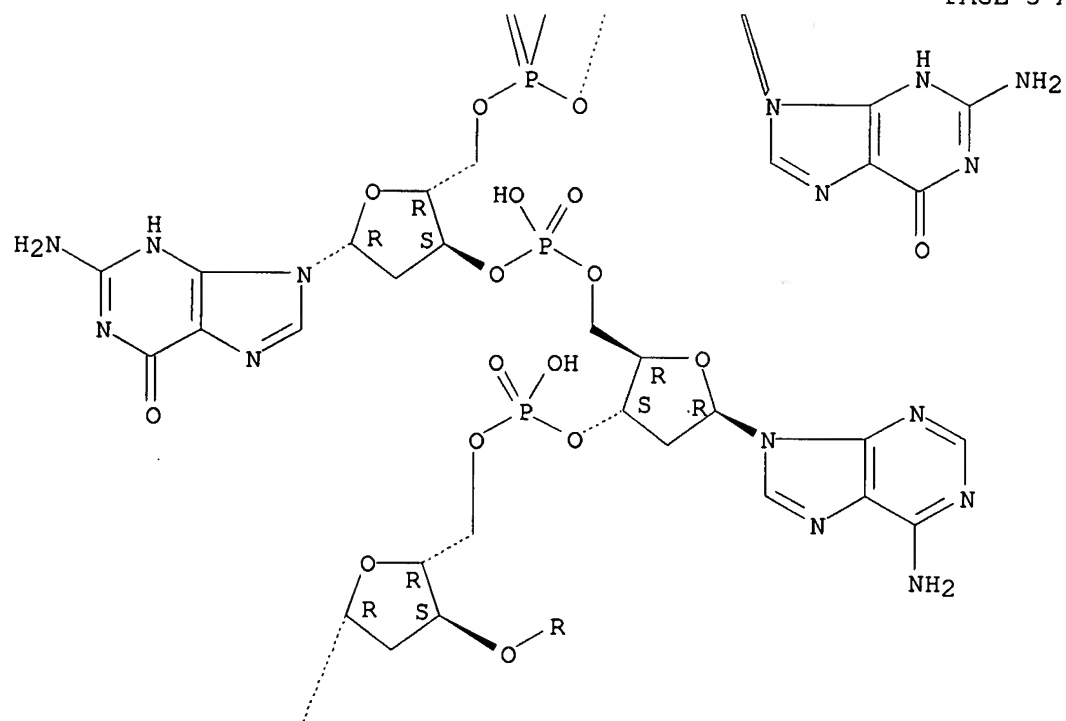
PAGE 2-A



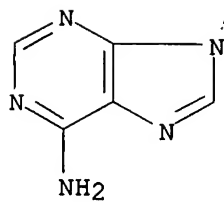
PAGE 2-B



PAGE 3-A



PAGE 4-A

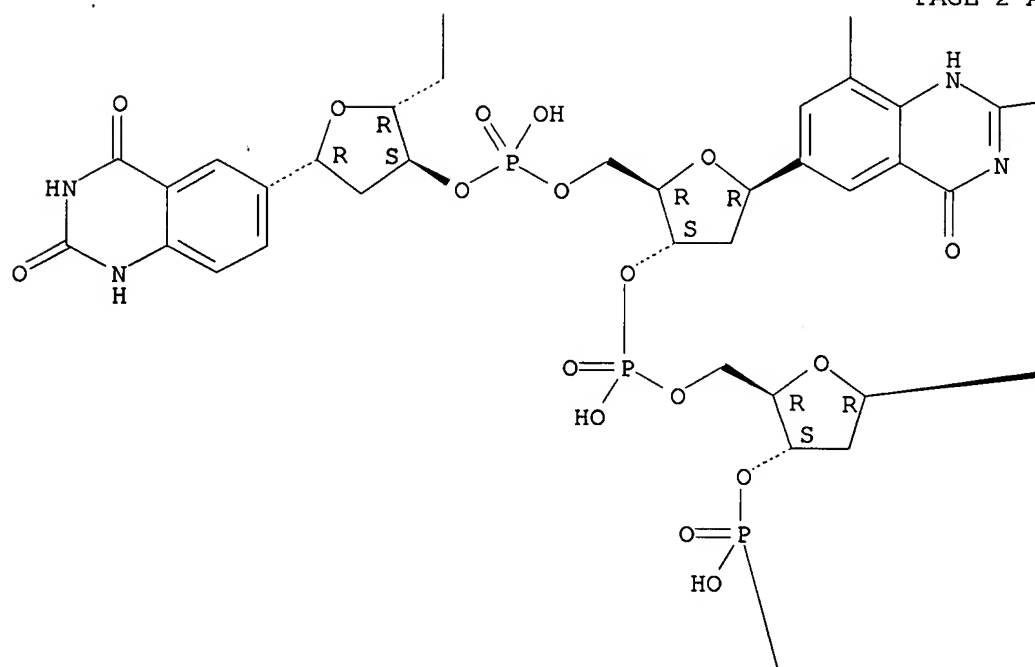
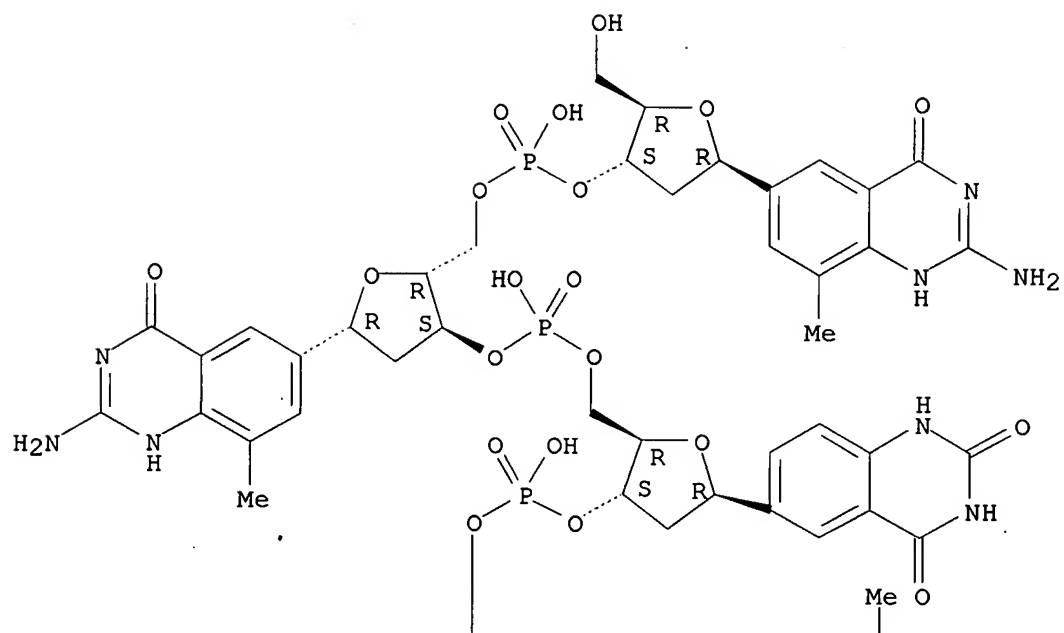


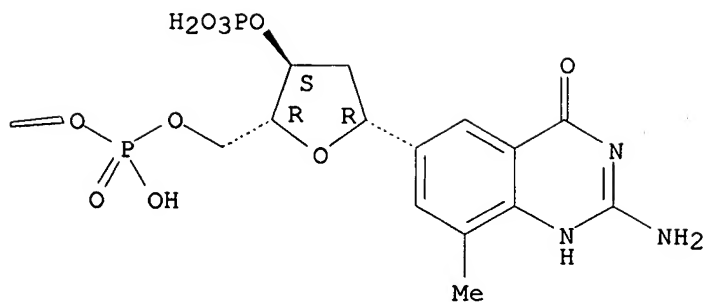
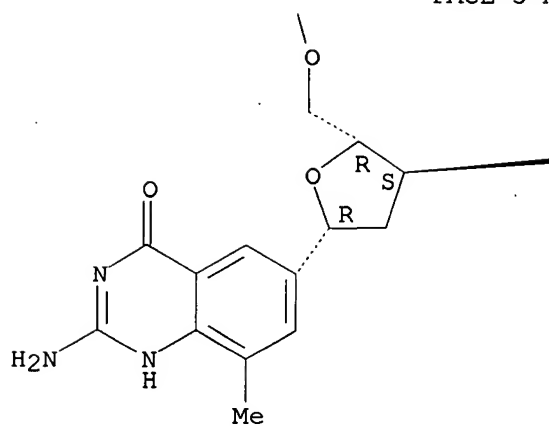
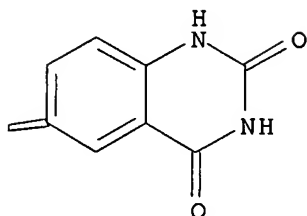
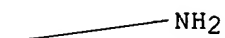
CM 2

CRN 850162-25-3

CMF C109 H121 N21 O52 P8

Absolute stereochemistry.





RN 850162-48-0 ZCAPLUS

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1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenyl-yl-(3'→5')-1'-(2-amino-
1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-

deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-, complex with guanylyl-(3'→5')-guanylyl-(3'→5')-adenylyl-(3'→5')-guanylyl-(3'→5')-adenylyl-(3'→5')-adenylyl-(3'→5')-guanylyl-(3'→5')-guanosine (1:1) (9CI) (CA INDEX NAME)

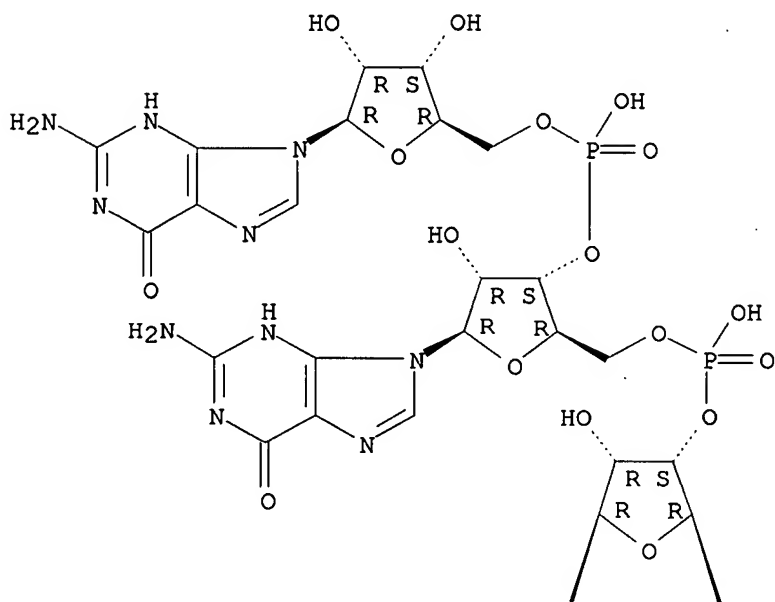
CM 1

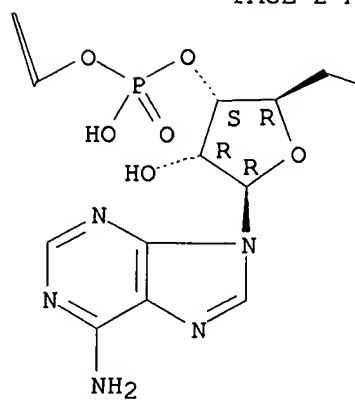
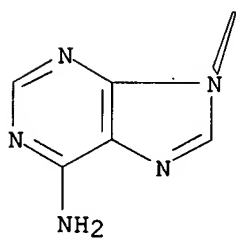
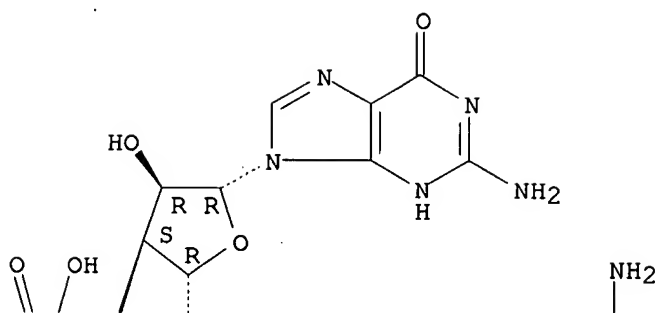
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CMF C80 H97 N40 O51 P7

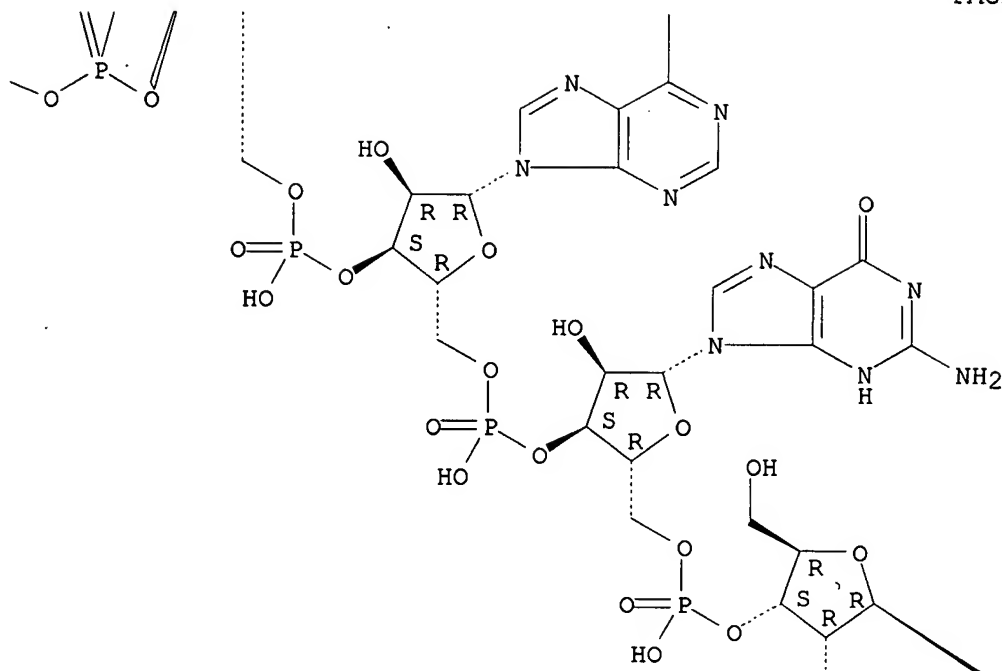
Absolute stereochemistry.

PAGE 1-A





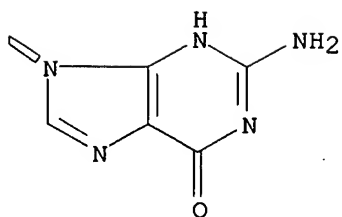
PAGE 2-B



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OH

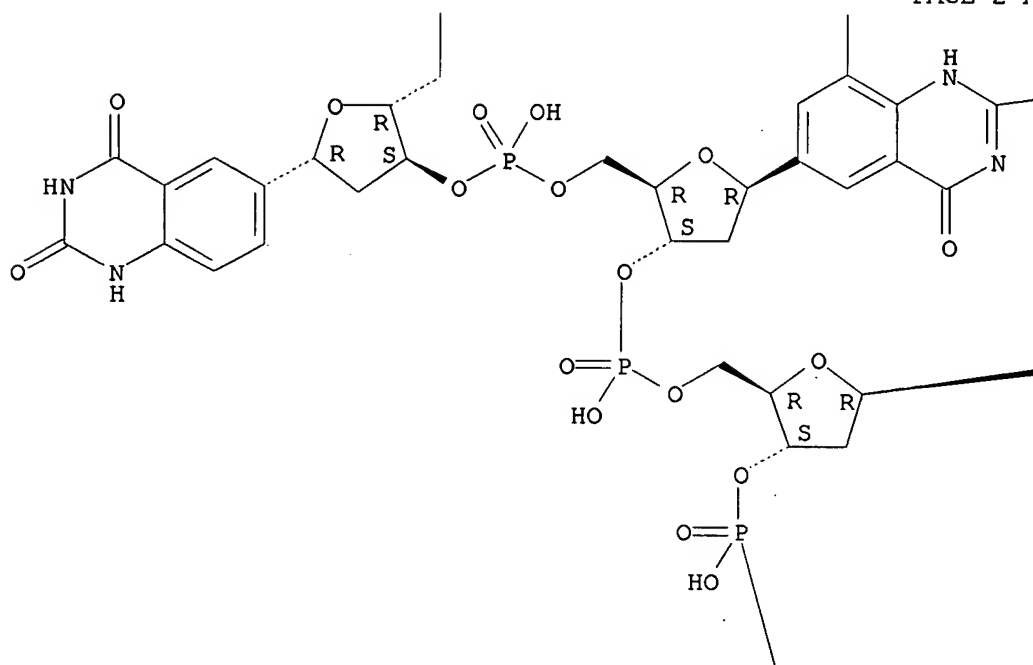
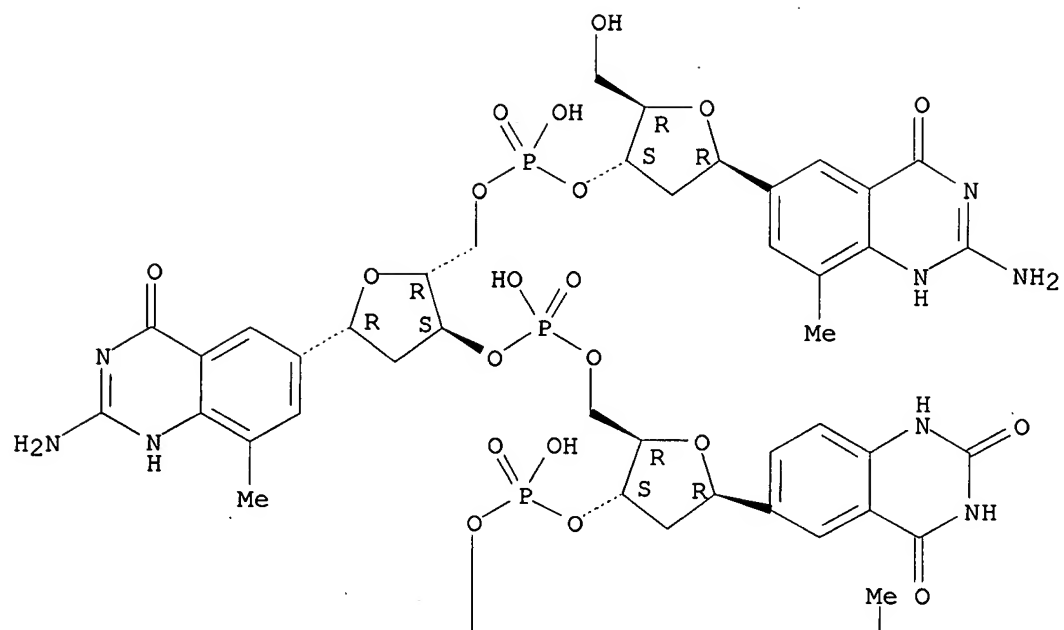
PAGE 3-C

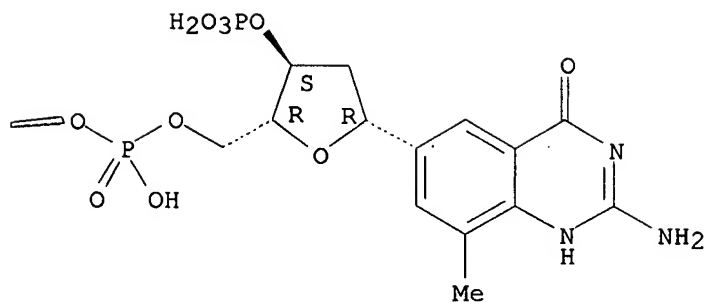
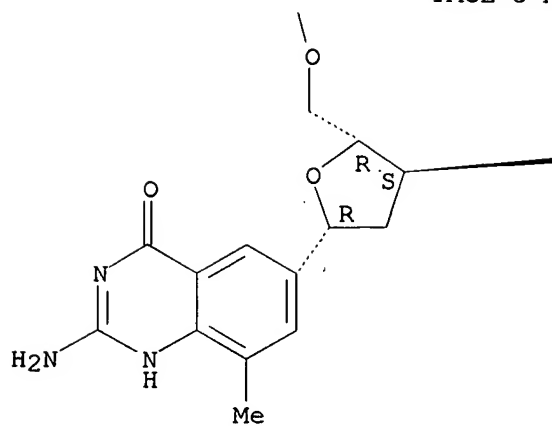
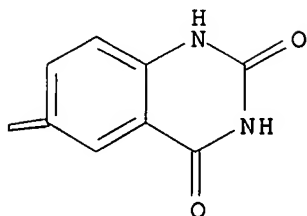
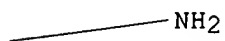


CM 2

CRN 850162-25-3
 CMF C109 H121 N21 O52 P8

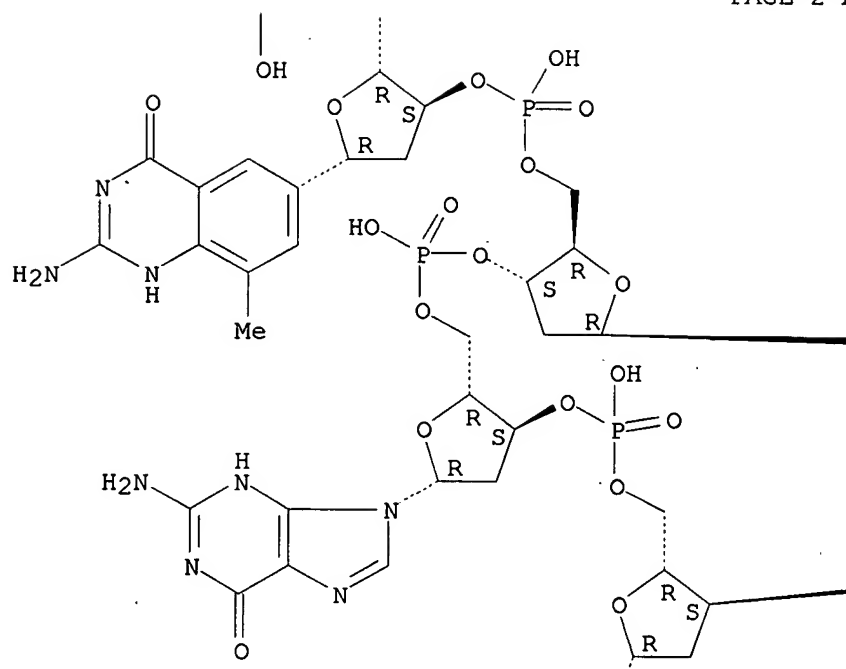
Absolute stereochemistry.



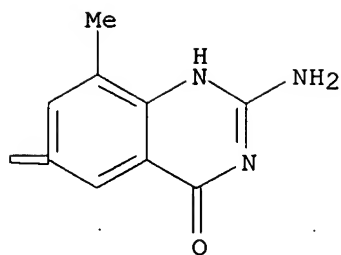


RN 850163-10-9 ZCAPLUS
 CN 3'-Guanylic acid, 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-
 1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenyl-yl-(3'→5')-1'-(2-amino-
 1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-

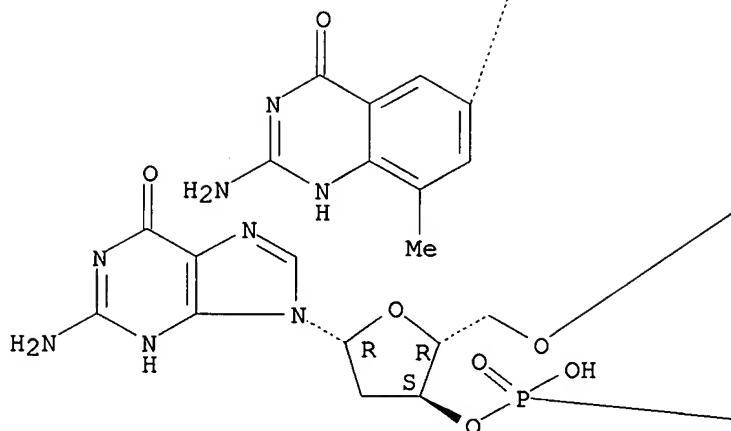
PAGE 2-A



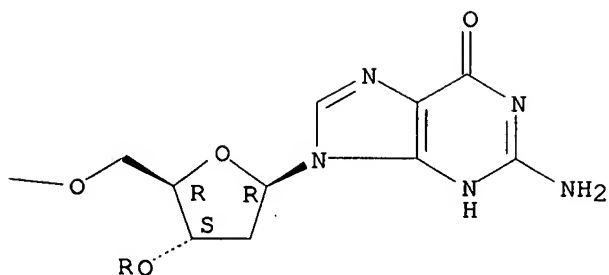
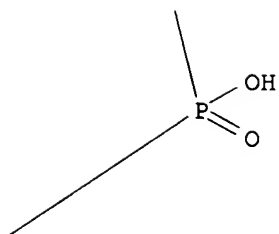
PAGE 2-B



PAGE 3-A



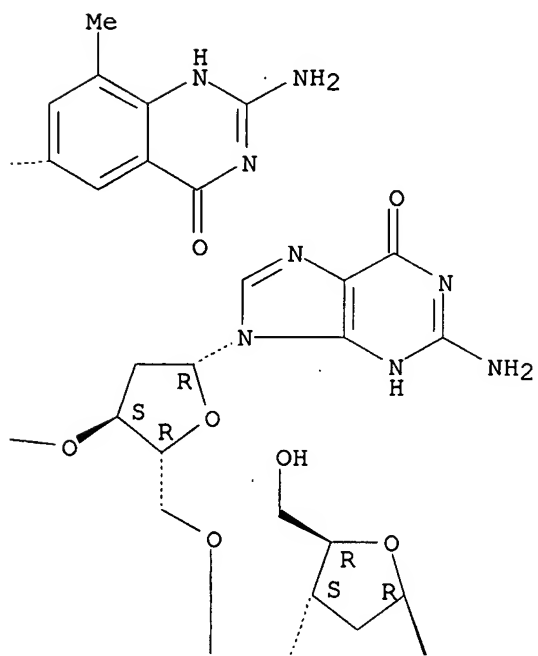
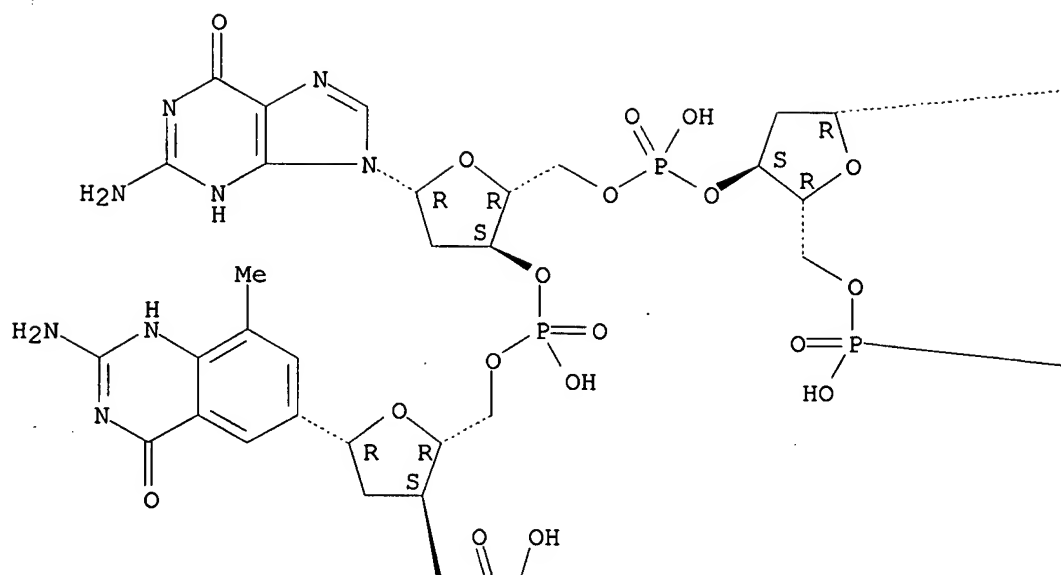
PAGE 3-B



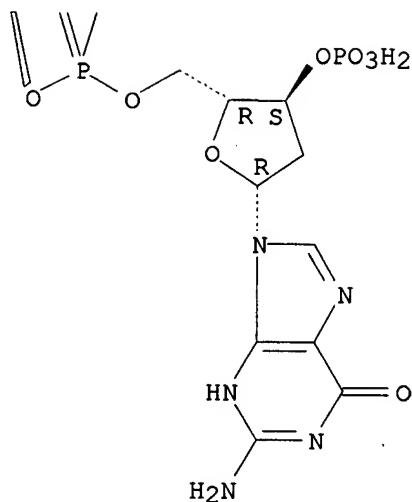
RN 850163-14-3 ZCAPLUS

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 1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-2'-
 deoxyguanylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
 quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-
 2'-deoxyguanylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-
 quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-
 2'-deoxy- (9CI) (CA INDEX NAME)

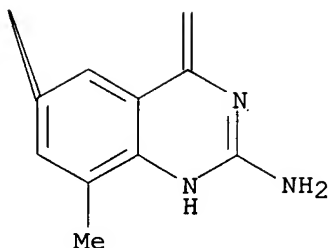
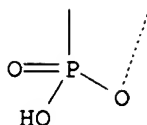
Absolute stereochemistry.



PAGE 2-A



PAGE 2-B



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2005:74697 ZCAPLUS

DOCUMENT NUMBER: 142:298070

TITLE: Quinazolinethiones and quinazolinethiones, novel inhibitors of inosine monophosphate dehydrogenase: synthesis and initial structure-activity relationships

AUTHOR(S): Buckley, George M.; Davies, Natasha; Dyke, Hazel J.; Gilbert, Philip J.; Hannah, Duncan R.; Haughan, Alan F.; Hunt, Caroline A.; Pitt, William R.; Profit, Rachael H.; Ray, Nicholas C.; Richard, Marianna D.; Sharpe, Andrew; Taylor, Alicia J.; Whitworth, Justine M.; Williams, Sophie C.

CORPORATE SOURCE: Celltech R&D, Cambridge, CB1 6GS, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 751-754

CODEN: BMCLE8; ISSN: 0960-894X

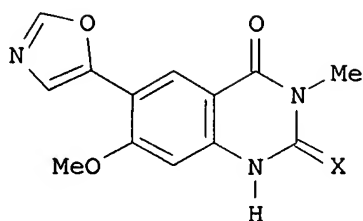
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:298070

GI



AB The development of a series of novel quinazolinethiones, e.g. I (X = S), and quinazolinediones, e.g. I (X = O), as inhibitors of inosine monophosphate dehydrogenase (IMPDH) is described. The synthesis, in vitro inhibitory values for IMPDH II and in vitro inhibitory value for PBMC proliferation are discussed.

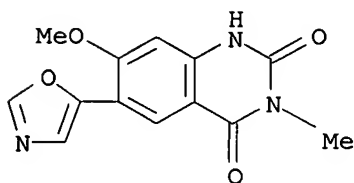
IT 847941-19-9P 847941-29-1P 847941-30-4P
847941-32-6P 847941-33-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and initial structure-activity relationships of quinazolinethiones and quinazolinediones, novel inhibitors of inosine monophosphate dehydrogenase)

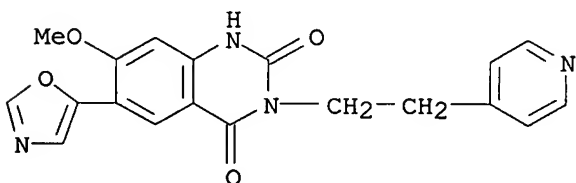
RN 847941-19-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-methoxy-3-methyl-6-(5-oxazolyl)- (9CI) (CA INDEX NAME)



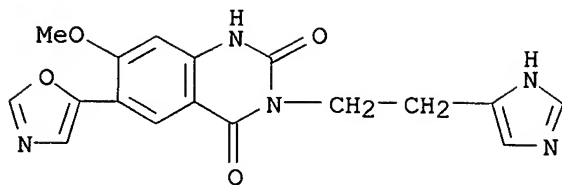
RN 847941-29-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-methoxy-6-(5-oxazolyl)-3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



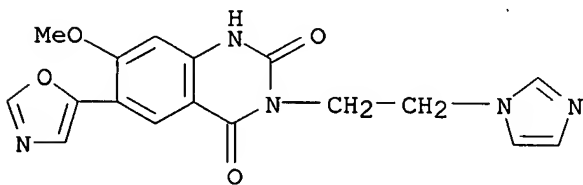
RN 847941-30-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-[2-(1H-imidazol-4-yl)ethyl]-7-methoxy-6-(5-oxazolyl)- (9CI) (CA INDEX NAME)



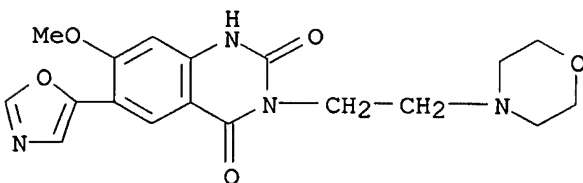
RN 847941-32-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 3-[2-(1H-imidazol-1-yl)ethyl]-7-methoxy-6-(5-oxazolyl)- (9CI) (CA INDEX NAME)



RN 847941-33-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 7-methoxy-3-[2-(4-morpholinyl)ethyl]-6-(5-oxazolyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1141805 ZCAPLUS

DOCUMENT NUMBER: 142:235099

TITLE: Size-Expanded Analogues of dG and dC: Synthesis and Pairing Properties in DNA

AUTHOR(S): Liu, Haibo; Gao, Jianmin; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA

SOURCE: Journal of Organic Chemistry (2005), 70(2), 639-647
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:235099

AB We describe the completion of the set of four benzo-fused expanded DNA (xDNA) nucleoside analogs. We previously reported the development of benzo-fused analogs of dA and dT and their inclusion in an exceptionally stable new four-base genetic system, termed xDNA, in which the base pairs were expanded in size. Here we describe the preparation and properties of the second half of this nucleotide set: namely, the previously unknown dxC and

dxG nucleosides. The dxC analog was prepared from the previously reported dxT nucleoside in three steps and 57% yield. The large-sized deoxyguanosine analog was prepared from an intermediate in the synthesis of dxA, yielding dxG in 14 steps overall (2.4%). Suitably protected versions of the deoxynucleosides were prepared for oligonucleotide synthesis following standard procedures, and they were readily incorporated into DNA by automated synthesizer. "Dangling-end" measurements revealed that the benzo-fused homologs stack considerably more strongly on neighboring DNA sequences than do their natural counterparts. Base pairing expts. with xC or xG bases showed that they pair selectively with their Watson-Crick partners, but with mild destabilization, due apparently to their larger size. Overall, the data suggest that the fluorescent xG and xC bases may be useful probes of steric effects in the study of biol. nucleotide recognition mechanisms. In addition, the completion of the xDNA nucleoside set makes it possible in the future to construct full four-base xDNA strands that can target any sequence of natural DNA and RNA.

IT 639465-38-6

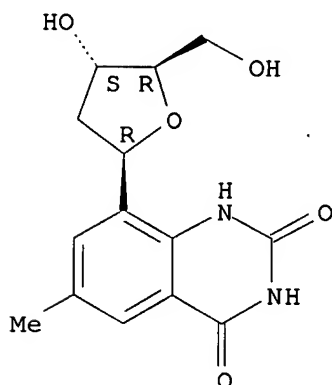
RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorescent xG and xC bases of xDNA may be useful probes of steric effects in study of biol. nucleotide recognition mechanisms)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 843639-18-9P

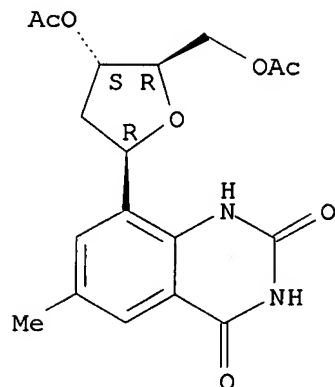
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorescent xG and xC bases of xDNA may be useful probes of steric effects in study of biol. nucleotide recognition mechanisms)

RN 843639-18-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 8-(3,5-di-O-acetyl-2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 28 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:1024090 ZCAPLUS
 DOCUMENT NUMBER: 142:198294
 TITLE: Novel Benzopyrimidines as Widened Analogs of DNA Bases
 AUTHOR(S): Lee, Alex H. F.; Kool, Eric T.
 CORPORATE SOURCE: Department of Chemistry, Stanford University,
 Stanford, CA, 94305, USA
 SOURCE: Journal of Organic Chemistry (2005), 70(1), 132-140
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:198294

AB We report on the synthesis, stacking, and pairing properties of a new structural class of size-expanded pyrimidine nucleosides, abbreviated dyT and dyC. Their bases are benzo-homologated variants of thymine and cytosine and have a design that is distinct from a previously described class of size-expanded (xDNA) pyrimidines, with a different vector of expansion relative to the sugar. We term this new base geometry "yDNA" (a mnemonic for "wide DNA"). Both C-glycosides were prepared using Pd-mediated coupling of iodinated base derivs. with a deoxyribose precursor. As free deoxynucleosides, both dyT and dyC displayed robust fluorescence, with emission maxima at 375 and 390 nm, resp. Both widened pyrimidines could be incorporated readily as protected phosphoramidite derivs. into synthetic oligonucleotides. Expts. in "dangling end" DNA contexts revealed that both yT and yC stack more favorably than their natural counterparts. When opposite natural bases in the context of Watson-Crick DNA were paired, the yT nucleotide formed a pair with A that was equally stable as a T-A pair, despite the mismatch in size with the neighboring natural pairs. The yC nucleotide (paired opposite G) was destabilizing by a small amount in the same context. Despite the large size of the pairs, both yT and yC were selective for their Watson-Crick complementary partners A and G, resp. The pairing properties and fluorescence of yDNA nucleotides may lead to useful applications in the study of steric effects in DNA-protein interactions. In addition, the compds. may serve as building blocks for a large-sized artificial genetic system.

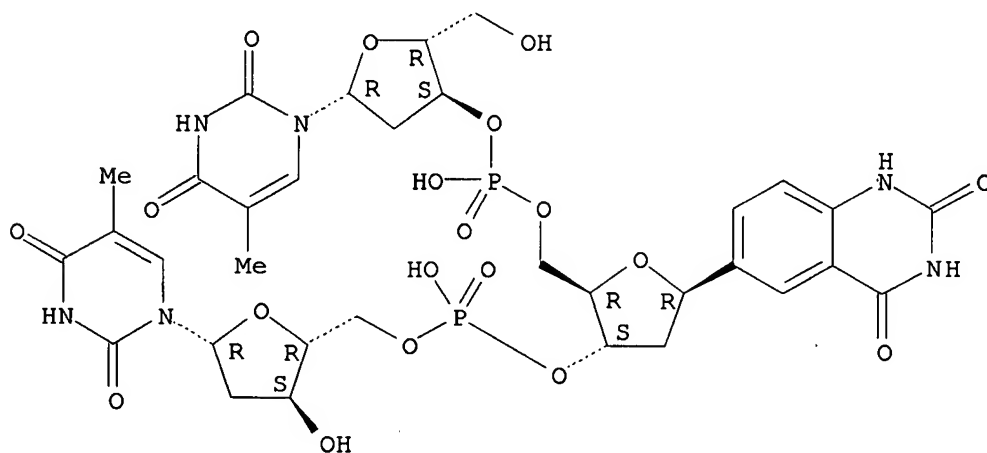
IT 830343-51-6P 830343-53-8P 830343-55-0P
 830343-57-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and thermodyn. of benzopyrimidines as widened analogs of DNA bases)

RN 830343-51-6 ZCAPLUS

CN Thymidine, thymidylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

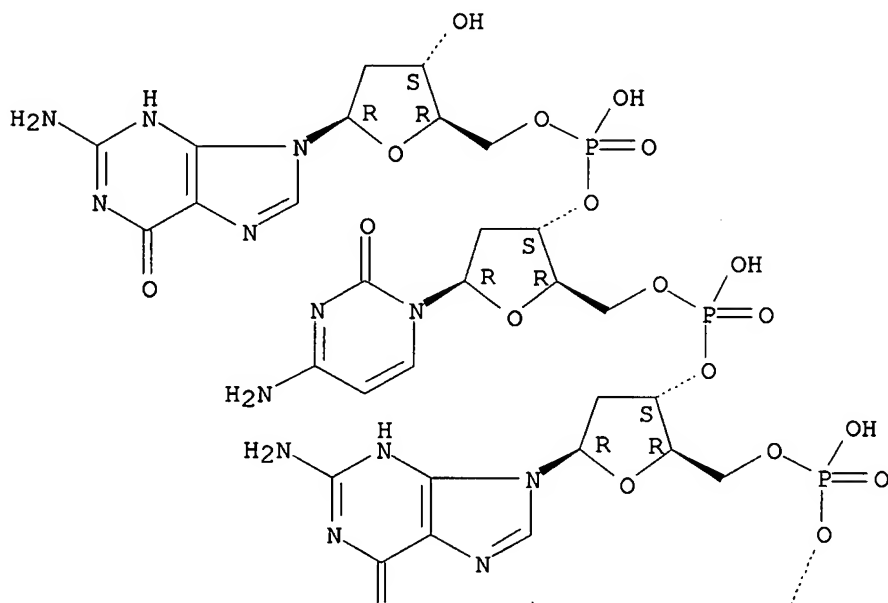


RN 830343-53-8 ZCAPLUS

CN Guanosine, 1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-2,4-dioxo-6-quinazolinyl)adenylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

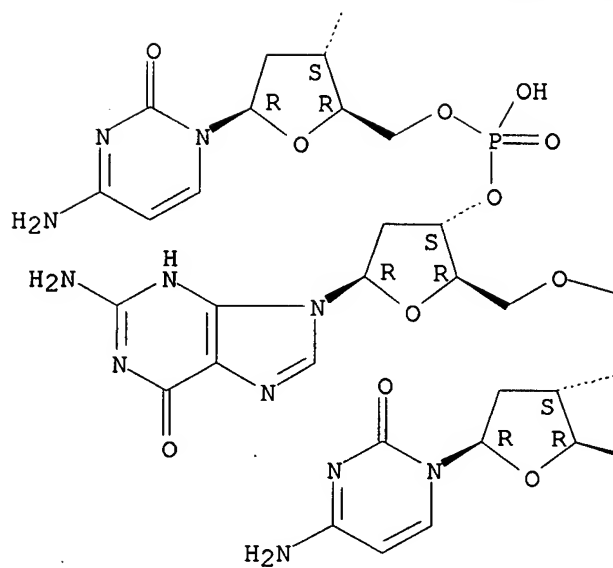
Absolute stereochemistry.

PAGE 1-A

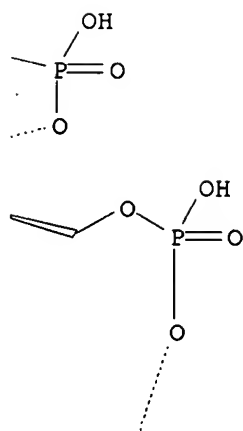


PAGE 2-A

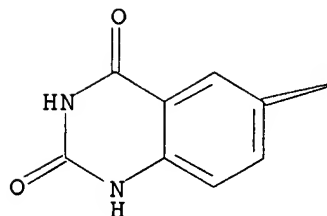
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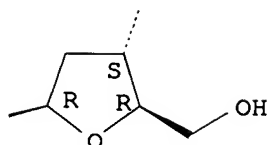
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PAGE 3-A



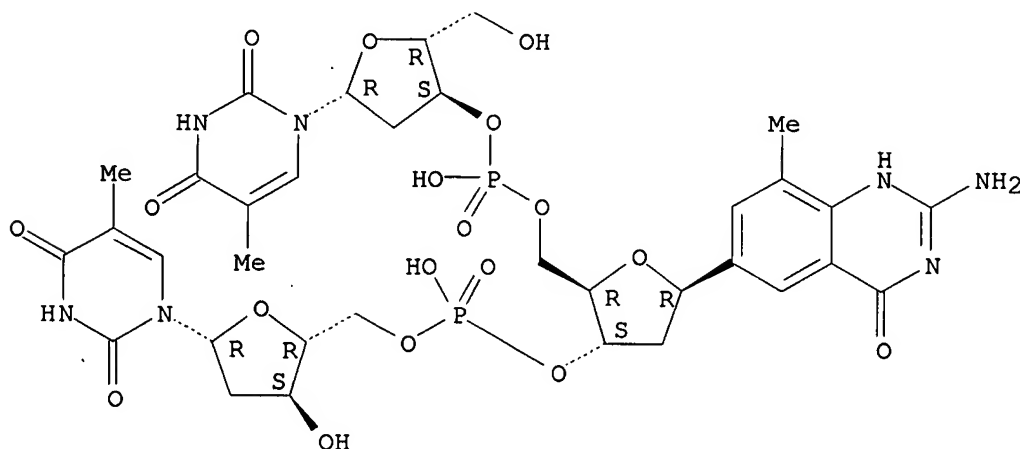
PAGE 3-B



RN 830343-55-0 ZCAPLUS

CN Thymidine, thymidylyl-(3'→5')-1'-(2-amino-1,4-dihydro-8-methyl-2,4-dioxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-(9CI) (CA INDEX NAME)

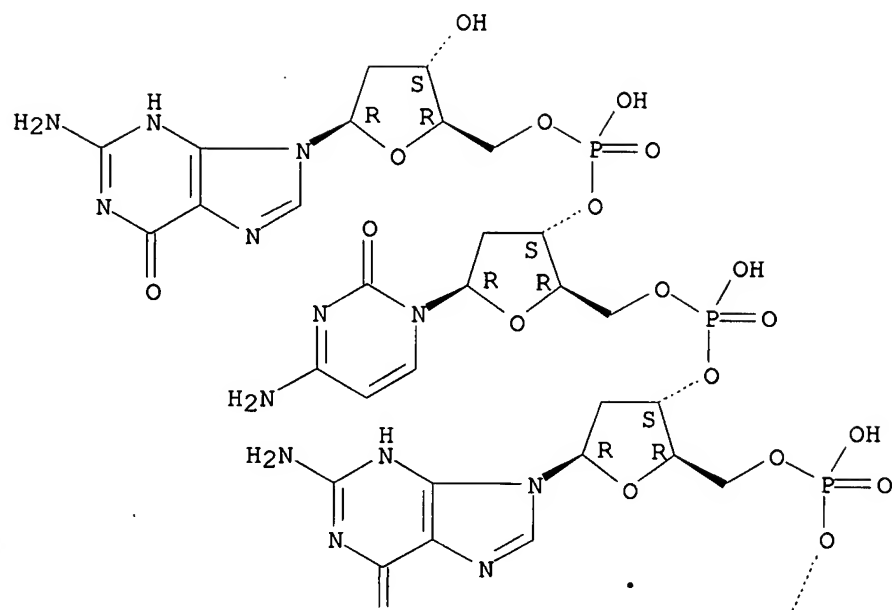
Absolute stereochemistry.



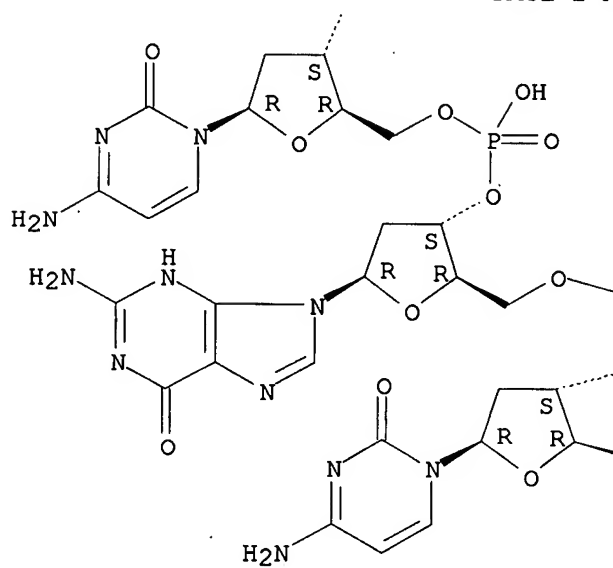
RN 830343-57-2 ZCAPLUS

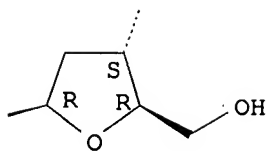
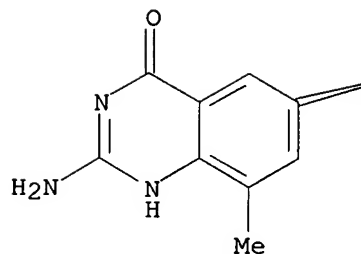
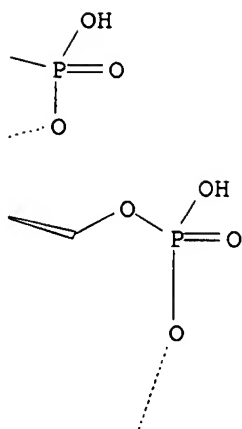
CN Guanosine, 1'-(2-amino-1,4-dihydro-8-methyl-4-oxo-6-quinazolinyl)-1'-de(6-amino-9H-purin-9-yl)-2'-deoxyadenylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



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IT 830343-47-0 830343-49-2

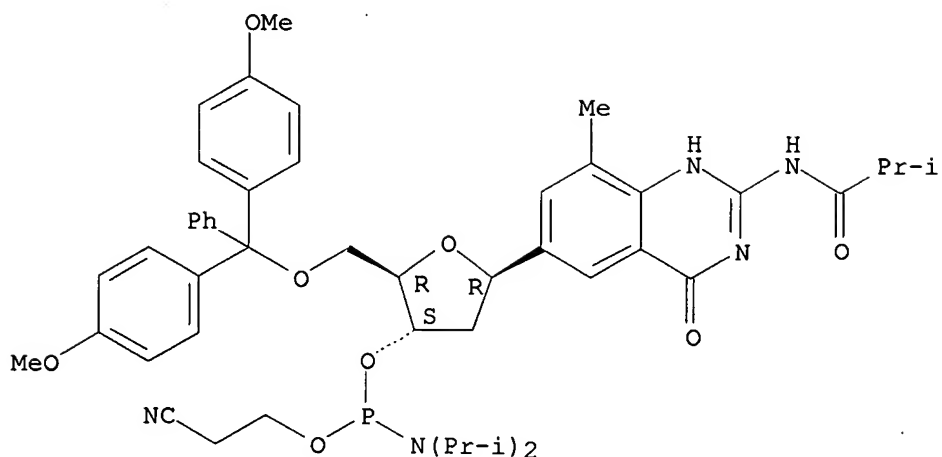
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and thermodyn. of benzopyrimidines as widened analogs of DNA bases)

RN 830343-47-0 ZCAPLUS

CN Propanamide, N-[6-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino](2-cyanoethoxy)phosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,4-dihydro-8-methyl-4-oxo-2-quinazolinyl]-2-methyl- (9CI)
(CA INDEX NAME)

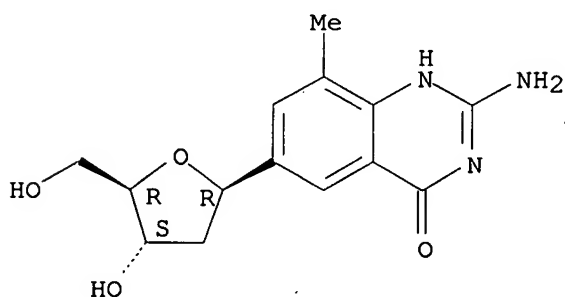
Absolute stereochemistry.



RN 830343-49-2 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-amino-6-(2-deoxy-β-D-erythro-pentofuranosyl)-8-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



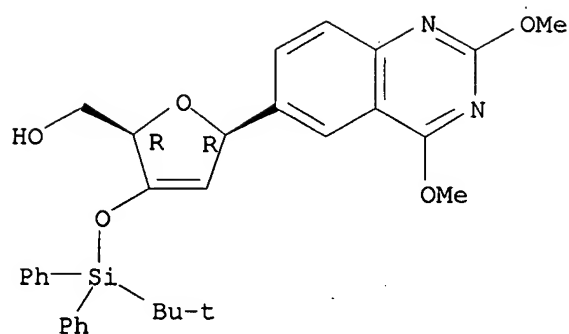
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830343-29-8P 830343-41-4P 830343-43-6P
830343-45-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermodyn. of benzopyrimidines as widened analogs of DNA bases)

RN 830343-17-4 ZCAPLUS

CN 2-Furanmethanol, 5-(2,4-dimethoxy-6-quinazolinyl)-3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2,5-dihydro-, (2R,5R)- (9CI) (CA INDEX NAME)

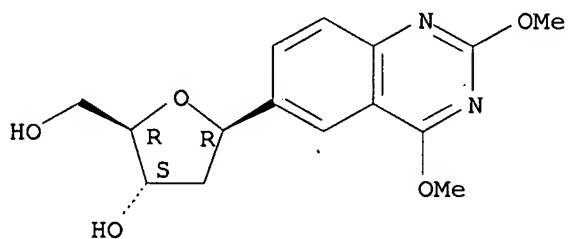
Absolute stereochemistry.



RN 830343-19-6 ZCAPLUS

CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-(2,4-dimethoxy-6-quinazolinyl)-, (1R)- (9CI) (CA INDEX NAME)

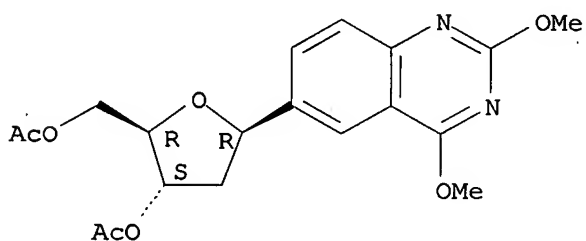
Absolute stereochemistry.



RN 830343-21-0 ZCAPLUS

CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-(2,4-dimethoxy-6-quinazolinyl)-, 3,5-diacetate, (1R)- (9CI) (CA INDEX NAME)

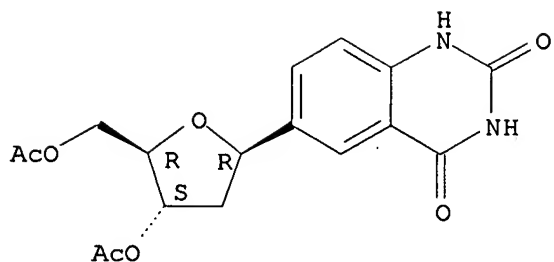
Absolute stereochemistry.



RN 830343-23-2 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(3,5-di-O-acetyl-2-deoxy-beta-D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

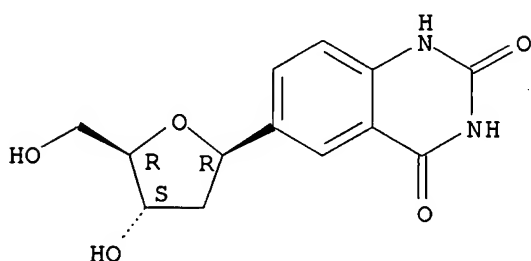
Absolute stereochemistry.



RN 830343-25-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(2-deoxy-β-D-erythro-pentofuranosyl)-
(9CI) (CA INDEX NAME)

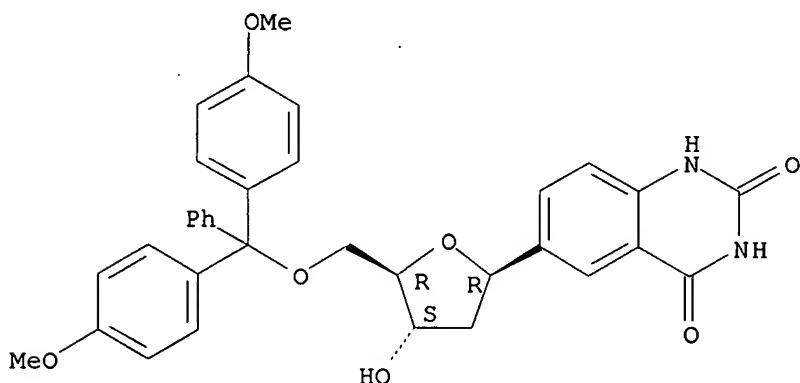
Absolute stereochemistry.



RN 830343-27-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)

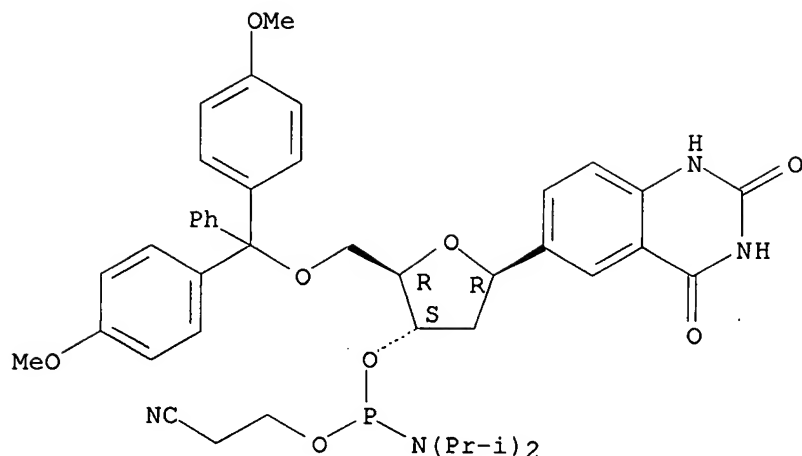
Absolute stereochemistry.



RN 830343-29-8 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino](2-cyanoethoxy)phosphino]-2-deoxy-β-D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)

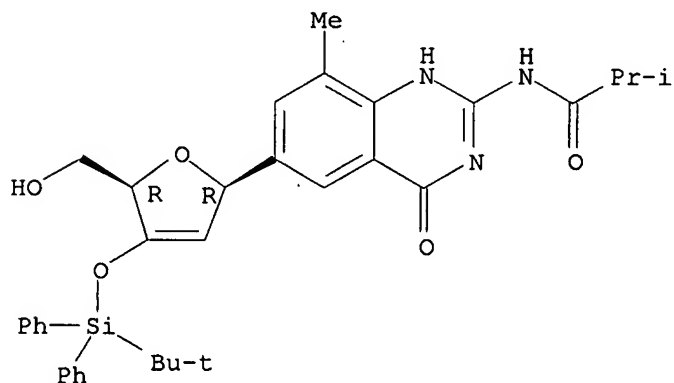
Absolute stereochemistry.



RN 830343-41-4 ZCAPLUS

CN Propanamide, N-[6-[(2R,5R)-4-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2,5-dihydro-5-(hydroxymethyl)-2-furanyl]-1,4-dihydro-8-methyl-4-oxo-2-quinazolinyl]-2-methyl- (9CI) (CA INDEX NAME)

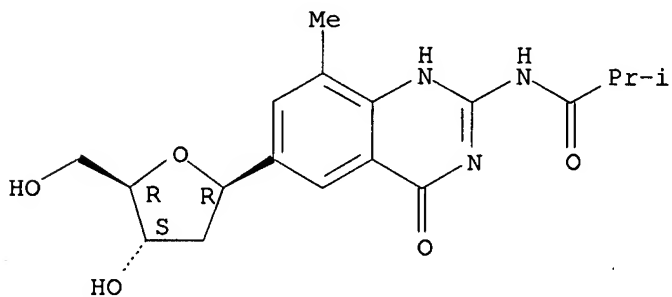
Absolute stereochemistry.



RN 830343-43-6 ZCAPLUS

CN Propanamide, N-[6-(2-deoxy-β-D-erythro-pentofuranosyl)-1,4-dihydro-8-methyl-4-oxo-2-quinazolinyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

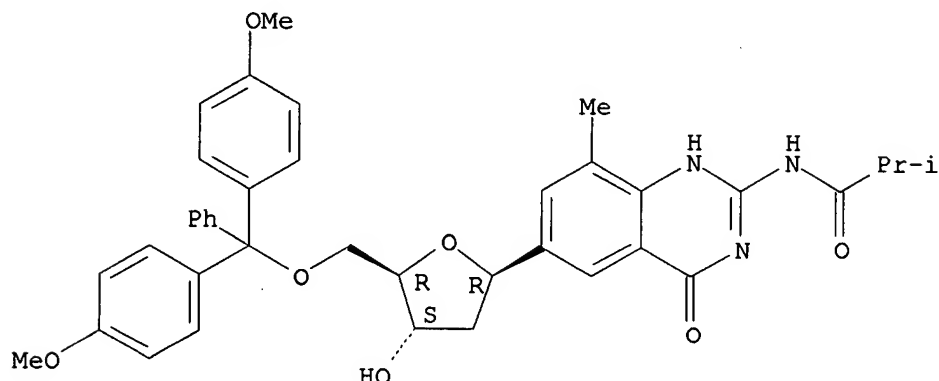


RN 830343-45-8 ZCAPLUS

CN Propanamide, N-[6-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-

erythro-pentofuranosyl]-1,4-dihydro-8-methyl-4-oxo-2-quinazolinyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:996140 ZCAPLUS

DOCUMENT NUMBER: 141:410954

TITLE: Preparation of substituted heteroaryls as inhibitors of protein tyrosine phosphatases for treatment of diabetes, cancer, and related conditions

INVENTOR(S): Savoy, Jennifer; Geraci, Leo; Parker, Garrett; Van Zandt, Michael C.; Whitehouse, Darren; Hu, Shaojing

PATENT ASSIGNEE(S): The Institutes for Pharmaceutical Discovery, LLC, USA

SOURCE: PCT Int. Appl., 124 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

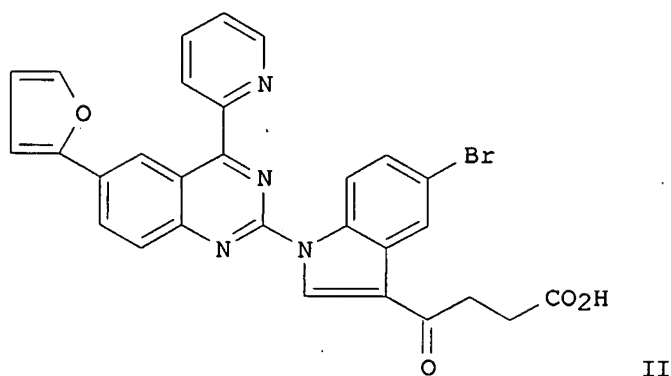
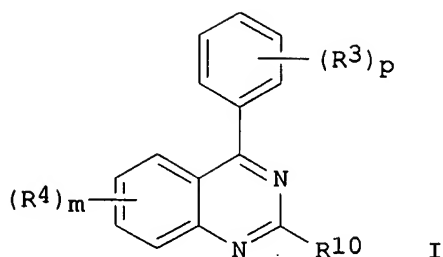
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
JP 2006525357	T	20061109	JP 2006-514209	20040430
PRIORITY APPLN. INFO.:			US 2003-466869P	P 20030430

OTHER SOURCE(S):
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MARPAT 141:410954

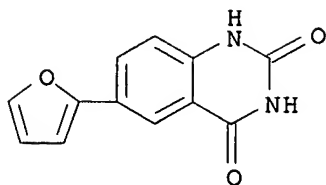


AB Disclosed are quinazolines I [wherein m = 0-4; n = 1-6; p = 0-5; q = 1-4; R1 = H, (carboxy)alkyl; R2 = (un)substituted Ph; R3 = independently halo, CN, OH, CO2R1, (un)substituted alkyl, alkoxy, CO(CH2)nCO2R1, (CH2)qOPh; R4 = independently halo, heteroaryl, haloalkyl, alkoxy, NO2, (un)substituted heterocyclyl; R10 = NR1R2, halo, (un)substituted (hetero)aryl, heterocyclyl; with provisos; and pharmaceutically acceptable salts thereof] and similarly substituted thiazoles, pyrimidines, and 1,3,5-triazines, which are useful in the treatment of metabolic disorders related to insulin resistance, leptin resistance, or hyperglycemia (no data). Compds. of the invention include inhibitors of protein tyrosine phosphatases, in particular protein tyrosine phosphatase-1B (PTP-1B), that are useful in the treatment of diabetes and other PTP mediated diseases, such as cancer, neurodegenerative diseases, and the like (no data). Also disclosed are pharmaceutical compns. comprising compds. of the invention and methods of treating the aforementioned conditions using such compds. For example, II was prepared in seven steps starting from 2-amino-5-bromobenzonitrile, 2-furanboronic acid, 2-pyridinylzinc bromide, and 4-(5-bromo-1H-indol-3-yl)-4-oxobutyric acid Me ester.

IT 792924-56-2P, 6-(Furan-2-yl)-1H-quinazoline-2,4-dione
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of substituted heteroaryls as PTP-1B inhibitors for treatment of diabetes, cancer, and related conditions)

RN 792924-56-2 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(2-furanyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 30 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:857326 ZCAPLUS

DOCUMENT NUMBER: 141:309639

TITLE: Dipeptidyl peptidase inhibitors

INVENTOR(S): Feng, Jun; Gwaltney, Stephen L.; Kaldor, Stephen W.;
Stafford, Jeffrey A.; Wallace, Michael B.; Zhang,
Zhiyuan

PATENT ASSIGNEE(S): Syrrx, Inc., USA

SOURCE: PCT Int. Appl., 244 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

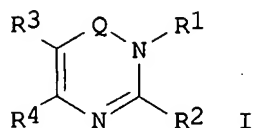
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087053	A2	20041014	WO 2004-US9217	20040324
WO 2004087053	A9	20041111		
WO 2004087053	A3	20060831		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2518465	A1	20041014	CA 2004-2518465	20040324
US 2004242568	A1	20041202	US 2004-809636	20040324
US 2004242566	A1	20041202	US 2004-809638	20040324
US 2004259870	A1	20041223	US 2004-809637	20040324
US 2005004117	A1	20050106	US 2004-809635	20040324
EP 1608317	A2	20051228	EP 2004-758366	20040324
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1894234	A	20070110	CN 2004-80011900	20040324
PRIORITY APPLN. INFO.:				
			US 2003-457785P	P 20030325
			WO 2004-US9217	W 20040324

OTHER SOURCE(S): MARPAT 141:309639

GI

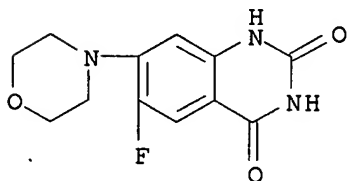


AB Dipeptidyl peptidase IV inhibitors I [Q = CO, SO, SO₂, C:NR₅; R₁ = ZR₆; Z = moiety providing 1-6 atom separation between R₆ and ring; R₂ = (substituted)3-7-membered ring; R₃,R₄ = taken together form a (substituted)5-6-membered ring; R₅ = H, (substituted)alkyl, cycloalkyl, etc.; R₆ = (substituted)C₃-7-cycloalkyl or aryl] are disclosed. Thus, 2-[2-(3-aminopiperidin-1-yl)-6,7-dimethoxy-4-oxo-4H-quinazolin-3-ylmethyl]benzonitrile (I; R₁ = 2-cyanophenylmethyl; R₂ = 3-aminopiperidin-1-yl; R₃,R₄ = dimethoxyphenyl) was synthesized. This compound exhibited enhanced stability in rat liver microsomes.

IT 769158-55-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (dipeptidyl peptidase inhibitors)

RN 769158-55-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-1-one, 6-fluoro-7-(4-morpholinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 31 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:707857 ZCAPLUS

DOCUMENT NUMBER: 141:375965

TITLE: Expanded-Size Bases in Naturally Sized DNA: Evaluation of Steric Effects in Watson-Crick Pairing

AUTHOR(S): Gao, Jianmin; Liu, Haibo; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA

SOURCE: Journal of the American Chemical Society (2004), 126(38), 11826-11831
 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe physicochem. properties in DNA of altered-size nucleobases that retain Watson-Crick analogous hydrogen-bonding ability. Size-expanded analogs of adenine and thymine (xA and xT, resp., which are expanded by benzo-fusion) were incorporated into natural DNA oligonucleotides, and their effects on helix stability were measured. Base stacking studies revealed that the two stretched analogs stack much more strongly than do their naturally sized counterparts. In contrast to this, pairing studies showed that single substitutions of the new bases are destabilizing to the natural helix as compared to A or T in standard A-T pairs in the same context, unless multiple adjacent substitutions are used. Interestingly, the size-expanded bases displayed selective recognition of the hydrogen-bonding complementary partners, suggesting

that Watson-Crick analogous pairs were still formed despite local backbone strain. In an attempt to compensate for the added size of the expanded adenine, we tested a formamide deoxynucleoside, which Leonard proposed as a shortened thymine analog (F0). Data showed, however, that this compound adopts a conformation unfavorable for pairing. On the basis of the combined thermodynamic data, we estimate the energetic cost of the 2.4 Å stretching of an isolated base pair in DNA at ca. +1 to 2 kcal/mol. Notably, during the pairing studies, the two size-expanded nucleobases were found to display significant changes in fluorescence on formation of stacked vs. unstacked structures, suggesting possible applications in probing nucleic acid structures and biochemical mechanisms.

IT 639465-38-6

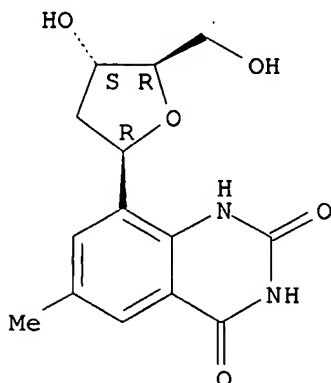
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(base pairing; expanded-size bases in naturally sized DNA and evaluation of steric effects in Watson-Crick pairing)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-6-one, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 781671-44-1

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

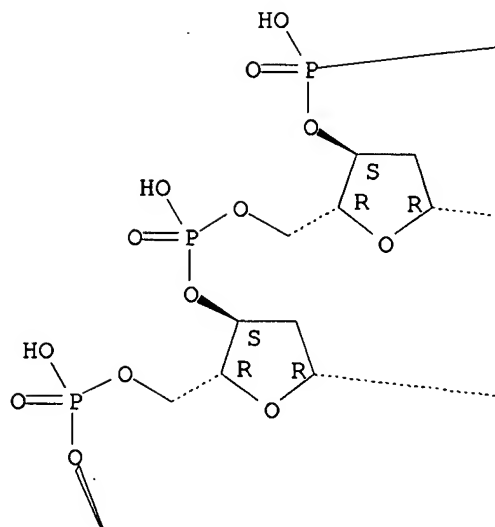
(expanded-size bases in naturally sized DNA and evaluation of steric effects in Watson-Crick pairing)

RN 781671-44-1 ZCAPLUS

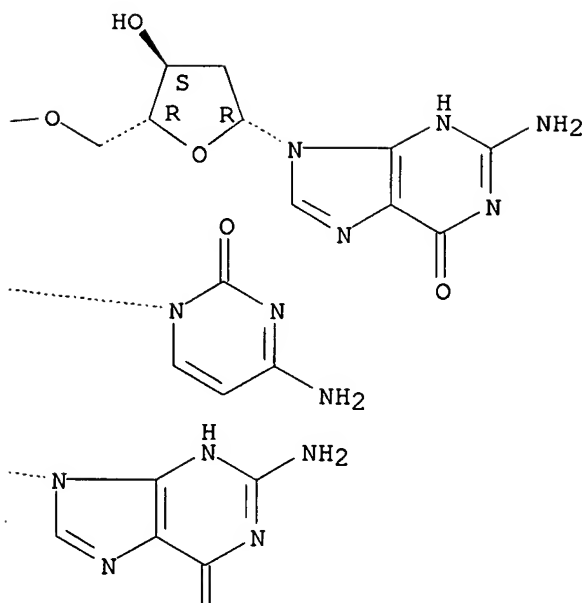
CN Guanosine, 1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-6-methyl-2,4-dioxo-8-quinazolinyl)adenylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

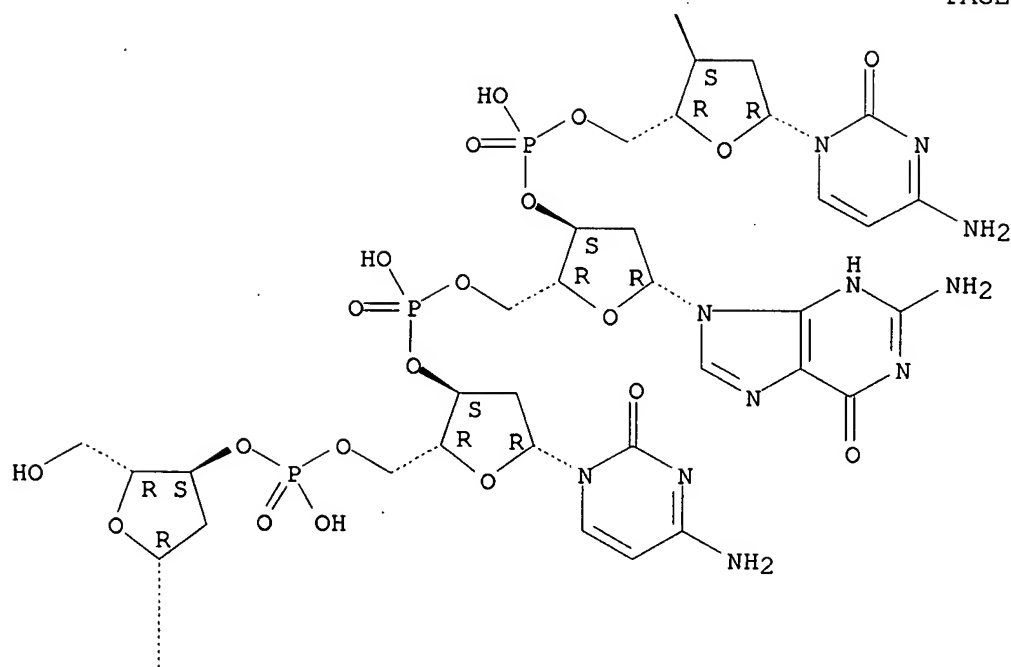
PAGE 1-A



PAGE 1-B



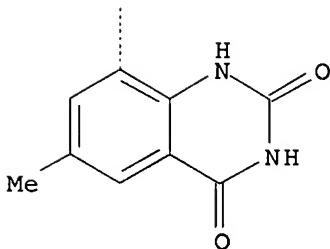
PAGE 2-A



PAGE 2-B



PAGE 3-A



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 32 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

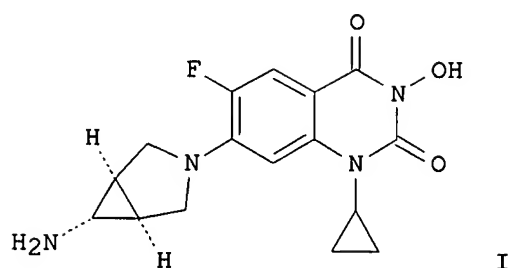
ACCESSION NUMBER: 2004:626167 ZCAPLUS

DOCUMENT NUMBER: 141:295972

TITLE: Synthesis and structural-activity relationships of 3-hydroxyquinazoline-2,4-dione antibacterial agents
 AUTHOR(S): Tran, Tuan P.; Ellsworth, Edmund L.; Stier, Michael A.; Domagala, John M.; Showalter, H. D. Hollis; Gracheck, Stephen J.; Shapiro, Martin A.; Joannides, Themis E.; Singh, Rajeshwar

CORPORATE SOURCE: Department of Chemistry, Pfizer Global Research and Development, Ann Arbor Laboratories, Ann Arbor, MI,

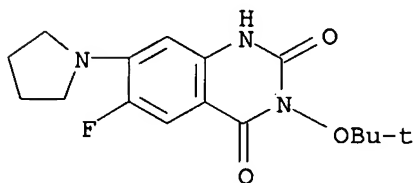
48105, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),
 14(17), 4405-4409
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:295972
 GI



AB A series of 3-hydroxyquinazoline-2,4-diones, e.g., I, was synthesized and evaluated for antibacterial activity. This series represents an addition to the DNA gyrate inhibitor class of antibacterials. Appropriated substitution onto the core template yielded compds. with excellent potency against E. coli gyrate and significant in vitro Gram-neg. and Gram-pos. antibacterial activity.

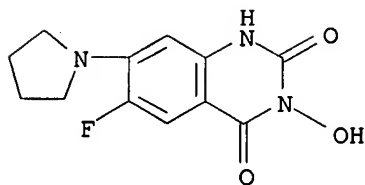
IT 761403-93-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, antibacterial activity, and structure-activity relationship of hydroxyquinazolinone via amidation of aminodifluorobenzoic acid with t-Bu hydroxylamine followed by heterocyclization, substitution, and hydrolysis)

RN 761403-93-4 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinone, 3-(1,1-dimethylethoxy)-6-fluoro-7-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



IT 224189-36-0P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, antibacterial activity, and structure-activity relationship of hydroxyquinazolinones via amidation of aminobenzoic acids with t-Bu hydroxylamine followed by heterocyclization, N-alkylation, substitution, and hydrolysis)

RN 224189-36-0 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinone, 6-fluoro-3-hydroxy-7-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 33 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:445389 ZCAPLUS

DOCUMENT NUMBER: 141:174142

TITLE: Synthesis of 4,5-diarylquinazolines: a system with cofacial aromatic rings. Diazines. Part 39

AUTHOR(S): Busch, Alexandrine; Gautheron Chapoulaud, Valerie; Audoux, Jerome; Ple, Nelly; Turck, Alain

CORPORATE SOURCE: Laboratoire de Chimie Organique Fine et Heterocyclique, UMR 6014, IRCOF-INSA, Mont Saint Aignan, 76131, Fr.

SOURCE: Tetrahedron (2004), 60(25), 5373-5382

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:174142

AB Using metalation reactions and Pd-catalyzed coupling, we report here two synthetic routes leading to eight new 4,5-di(hetero)arylquinazolines. Non-linear activity has been highlighted for some of these compds. with stacked aromatic rings.

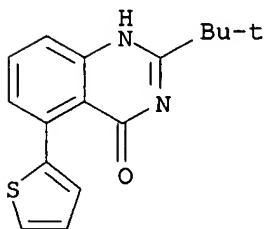
IT 733017-22-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diarylquinazolines via cross-coupling reaction and metalation)

RN 733017-22-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-(1,1-dimethylethyl)-5-(2-thienyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 34 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

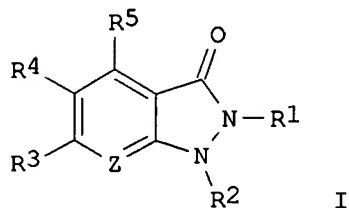
ACCESSION NUMBER: 2004:370926 ZCAPLUS

DOCUMENT NUMBER: 140:391292

TITLE: Preparation of indazolinone compositions useful as kinase inhibitors

INVENTOR(S): Aronov, Alex; Lauffer, David J.; Li, Huan Qui;
 Tomlinson, Ronald Charles; Li, Pan
 PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
 SOURCE: PCT Int. Appl., 260 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

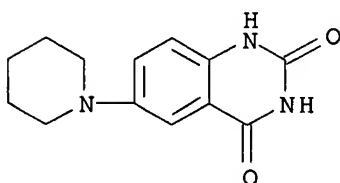
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037814	A1	20040506	WO 2003-US34065	20031027
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003286711	A1	20040513	AU 2003-286711	20031027
US 2004167121	A1	20040826	US 2003-694534	20031027
PRIORITY APPLN. INFO.:			US 2002-421398P	P 20021025
			WO 2003-US34065	W 20031027
OTHER SOURCE(S):		MARPAT 140:391292		
GI				



AB The present invention provides compds. of formula (I). [Wherein R1, R2 = H or a nitrogen protecting group; one of R3 or R4 = R and the other one of R3 or R4 = -Q1-A-Q2-Y; wherein Q1 = a valence bond, NRa, C(Ra)2, S, O, SO2, NRaSO2, SO2NRa, CO, NRaCO, CONRa, OC(O), C(O)O, OC(O)NRa, 1,2-cyclopropanedilyl, 1,2-cyclobutanediyl, or 1,3-cyclobutanediyl, optionally substituted C2-4 alkylidene, etc.; wherein Ra = H, each optionally substituted C1-4 aliphatic; A = optionally substituted 5-to 7-membered monocyclic or 8- to 10-membered bicyclic aryl, heteroaryl, heterocyclic, carbocyclic ring, or C2-6 alkylidene, etc.; Q2 = NRc, SO, O, or C(Rc)2; wherein Rc = H, optionally substituted C1-4 aliphatic; Y = each optionally substituted 5- to 7-membered monocyclic or 8- to 10 membered bicyclic aryl, heteroaryl, heterocyclic, or carbocyclic ring; R5 = R; Z = N, CR6; wherein R6 = R; R = H, halo, Q-halogen, cyano, Q-CN, NO2, Q-NO2, R7, Q-R7; Q = optionally substituted C1-4 alkylidene; wherein one or more methylene units of Q is optionally replaced by O, S, NR7, NR7CO, NR7CONR7, NR7CO2, CO, CO2, CONR7, OC(O)NR7, SO2, SO2NR7, NR7SO2, NR7SO2NR7, C(O)C(O), or C(O)C(R7)2C(O); wherein R7 = H, each optionally substituted aliphatic, heteroaliph., aryl or heteroaryl]. The compds. I and pharmaceutically acceptable compns. thereof, are useful generally as protein kinase inhibitors, particularly as inhibitors of protein kinase

PRAK, protein kinase GSK3, protein kinase ERK2, protein kinase CDK2, MAP kinase-activated protein kinase 2 (MK2), SRC kinase, protein kinase SYK, and protein kinase Aurora-2. Accordingly, the compds. I and compns. of the invention are useful for treating or lessening the severity of a disease or condition selected from cardiovascular disease, diabetes, neurol. disorders (e.g. Alzheimer's disease), immunodeficiency disorders, inflammatory diseases, allergic diseases, autoimmune diseases, destructive bone disorders such as osteoporosis, proliferative disorders, infectious diseases, and viral diseases. Thus, a solution of (2-chloroquinazolin-4-yl)(5-cyclopropyl-1H-pyrazol-3-yl)amine (50.0 mg, 0.175 mmol) and 6-amino-3-oxo-2,3-dihydroindazole-1-carboxylic acid tert-Bu ester (69.8 mg, 0.280 mmol) in NMP (1.0 mL) was heated up to 100° for 6 h to give, after workup, acidification with CF₃CO₂H, and HPLC purification, 6-[[4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]quinazolin-2-yl]amino]-1,2-dihydroindazol-3-one trifluoroacetate. Some compds. of the formula I were shown to have Ki of <0.1 µM for GSK-3 and Aurora-2 and <1.0 µM for CDK-2, ERK2, PRAK, SRC, SYK, and MK2.

IT 96086-60-1P, 6-(Piperidin-1-yl)-1H-quinazoline-2,4-dione
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of indazolinone derivs. as kinase inhibitors for treating or lessening severity of diseases or conditions)
 RN 96086-60-1 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolidinedione, 6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



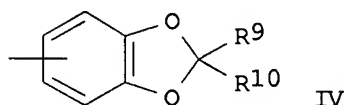
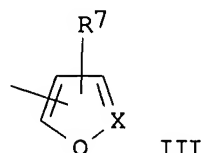
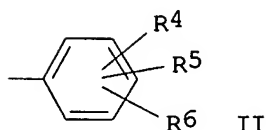
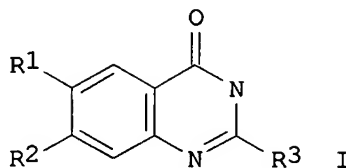
L4 ANSWER 35 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:333702 ZCAPLUS
 DOCUMENT NUMBER: 140:357365
 TITLE: Preparation of quinazolinones as anti-hyperalgesic agents
 INVENTOR(S): Culshaw, Andrew James; Dziadulewicz, Edward Karol; Hallett, Allan; Hart, Terance William
 PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH
 SOURCE: PCT Int. Appl., 40 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004033435	A1	20040422	WO 2003-EP11276	20031010
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE,				

DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE,
SI, SK, TR

CA 2501529	A1	20040422	CA 2003-2501529	20031010
AU 2003273989	A1	20040504	AU 2003-273989	20031010
EP 1554257	A1	20050720	EP 2003-757959	20031010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014557	A	20050809	BR 2003-14557	20031010
CN 1711249	A	20051221	CN 2003-80102932	20031010
JP 2006503875	T	20060202	JP 2004-542493	20031010
US 2006154942	A1	20060713	US 2006-530897	20060309
PRIORITY APPLN. INFO.:			GB 2002-23730	A 20021011
OTHER SOURCE(S):			WO 2003-EP11276	W 20031010
GI			MARPAT 140:357365	

Pg
Pub.



AB The title compds. [I; R1 = halo, II-IV; X = N, CR8; R2 = halo, NO2, alkylcarbonyl, alkyl, cycloalkyl; R3 = alkyl, alkoxy, NH2; R4 = H, halo, OH, etc.; R5, R6 = H, halo, alkoxy, alkyl; R7, R8 = H, alkyl; R9, R10 = H, halo] which exhibit human vanilloid antagonistic activity, were prepared and formulated. Thus, a multi-step synthesis of 6-(4-chloro-3-cyclopropylmethoxyphenyl)-7-isopropyl-2-methyl-3H-quinazolin-4-one, starting from 2-nitro-4-cymene, was given. The compds. I effectively block Ca-uptake in the range from about 1 nM to about 10 μ M in fluorescence assay using CHO cells expressing human VR1 ion channels.

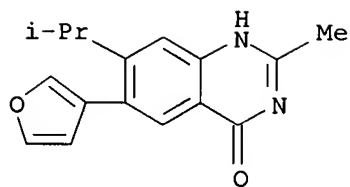
IT 681292-11-5P 681292-14-8P 681292-15-9P
681292-21-7P 681292-24-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazolinones as anti-hyperalgesic agents)

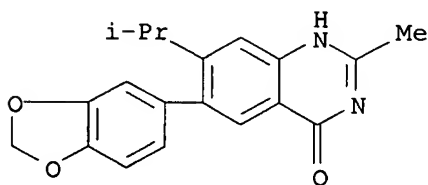
RN 681292-11-5 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-(3-furanyl)-2-methyl-7-(1-methylethyl)- (9CI) (CA INDEX NAME)



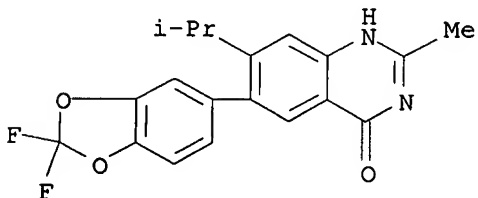
RN 681292-14-8 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-(1,3-benzodioxol-5-yl)-2-methyl-7-(1-methylethyl)-
(9CI) (CA INDEX NAME)



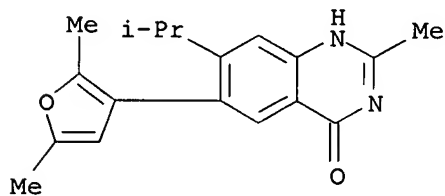
RN 681292-15-9 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-(2,2-difluoro-1,3-benzodioxol-5-yl)-2-methyl-7-(1-methylethyl)-
(9CI) (CA INDEX NAME)



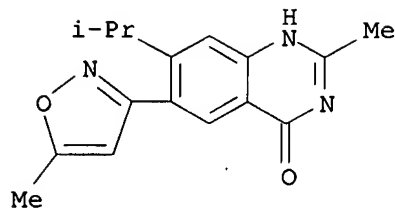
RN 681292-21-7 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-(2,5-dimethyl-3-furanyl)-2-methyl-7-(1-methylethyl)-
(9CI) (CA INDEX NAME)



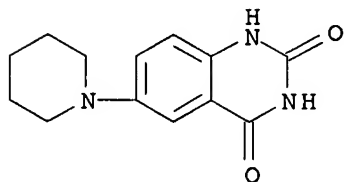
RN 681292-24-0 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-methyl-7-(1-methylethyl)-6-(5-methyl-3-isoxazolyl)-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 36 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:205966 ZCAPLUS
 DOCUMENT NUMBER: 142:197901
 TITLE: Product class 13: quinazolines
 AUTHOR(S): Kikelj, D.
 CORPORATE SOURCE: Germany
 SOURCE: Science of Synthesis (2004), 16, 573-749
 CODEN: SSCYJ9
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English
 AB A review. Preparation of quinazolines by ring closure and ring transformation reactions as well as aromatization and substituent modification is given.
 IT 96086-60-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of quinazolines)
 RN 96086-60-1 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinedione, 6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1014 THERE ARE 1014 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 37 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:45723 ZCAPLUS
 DOCUMENT NUMBER: 140:235993
 TITLE: Toward a New Genetic System with Expanded Dimensions: Size-Expanded Analogs of Deoxyadenosine and Thymidine
 AUTHOR(S): Liu, Haibo; Gao, Jianmin; Maynard, Lystranne; Saito, Y. David; Kool, Eric T.
 CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA
 SOURCE: Journal of the American Chemical Society (2004), 126(4), 1102-1109
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:235993

AB We describe the design, preparation, and properties of two key building blocks of a size-expanded genetic system. Nucleoside analogs of the natural nucleosides dA and dT are reported in which the fusion of a benzo ring increases their size by ca. 2.4 Å. The expanded dA analog (dxA), having a tricyclic base, was first reported by Leonard nearly three decades ago. We describe a shortened and more efficient approach to this compound. The expanded dT analog (dxT), a methylquinazolininedione C-glycoside, was previously unknown; we describe its preparation in eight steps from 5-methylanthranilic acid. The key glycoside bond formation employed Pd-mediated coupling of an aryl iodide precursor with a dihydrofuran derivative of deoxyribose. Both nucleosides are shown to be efficient fluorophores, emitting light in the blue-violet range. The base-protected phosphoramidite derivs. were prepared, and short oligonucleotides containing them were characterized. The two size-expanded nucleosides are key components of a new four-base genetic system designed to form helical paired structures having a diameter greater than that of natural DNA. Elements of the design of this expanded genetic mol., termed xDNA, are discussed, including the possibility of up to eight base pairs of information storage capability.

IT 639465-38-6P 667916-42-9P 667916-43-0P

667916-44-1P 667916-45-2P 667916-46-3P

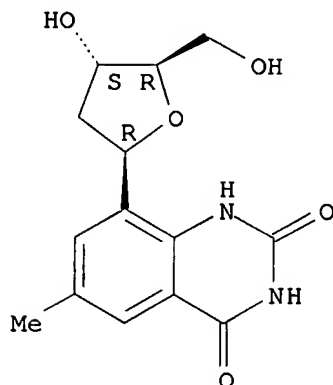
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and characterization of size-expanded analogs of deoxyadenosine and thymidine for use in genetic system with expanded dimensions)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolininedione, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

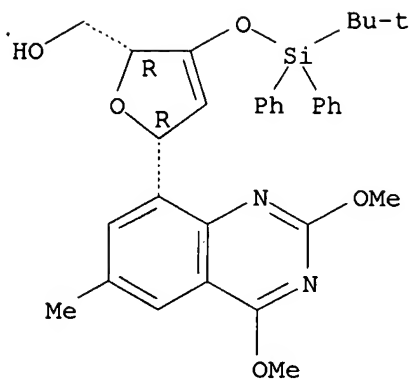
Absolute stereochemistry.



RN 667916-42-9 ZCAPLUS

CN 2-Furanmethanol, 5-(2,4-dimethoxy-6-methyl-8-quinazolinyl)-3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2,5-dihydro-, (2R,5R)- (9CI) (CA INDEX NAME)

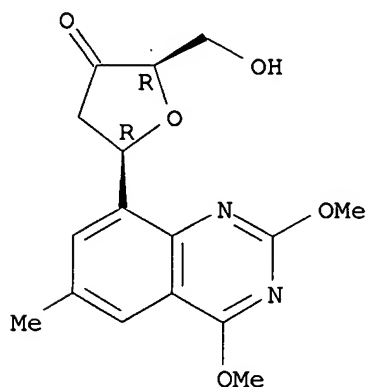
Absolute stereochemistry.



RN 667916-43-0 ZCAPLUS

CN 3(2H)-Furanone, 5-(2,4-dimethoxy-6-methyl-8-quinazolinyl)dihydro-2-(hydroxymethyl)-, (2R,5R)- (9CI) (CA INDEX NAME)

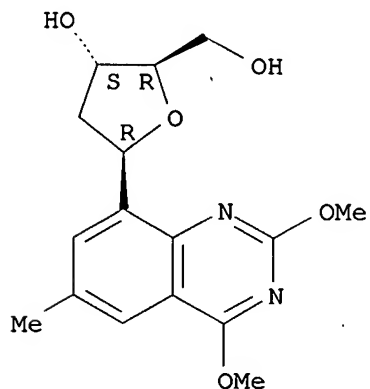
Absolute stereochemistry.



RN 667916-44-1 ZCAPLUS

CN Quinazoline, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-2,4-dimethoxy-6-methyl- (9CI) (CA INDEX NAME)

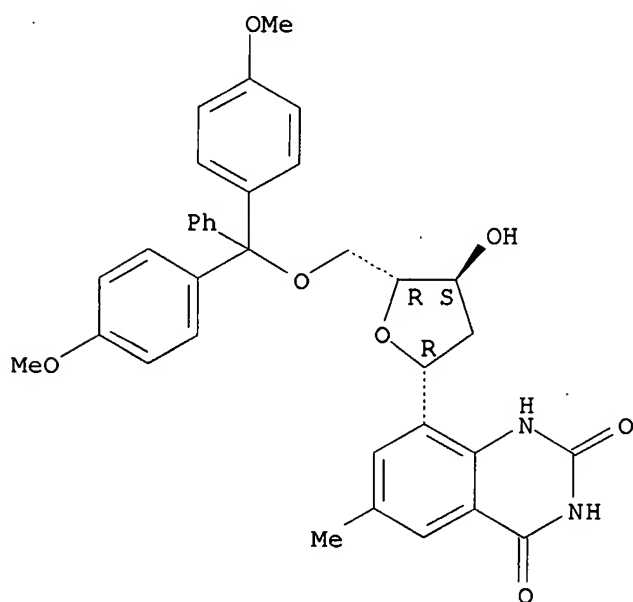
Absolute stereochemistry.



RN 667916-45-2 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 8-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-6-methyl- (9CI) (CA INDEX NAME)

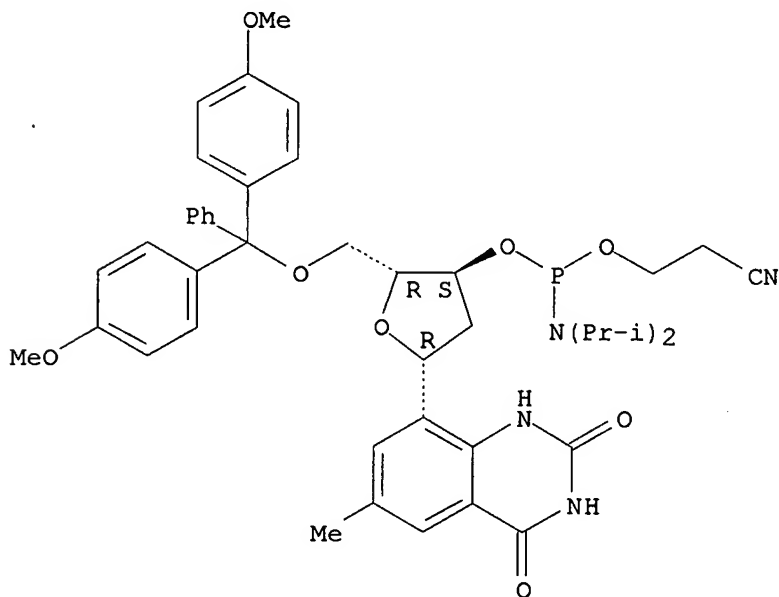
Absolute stereochemistry.



RN 667916-46-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 8-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino](2-cyanoethoxy)phosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-6-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 667916-48-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and characterization of size-expanded analogs of

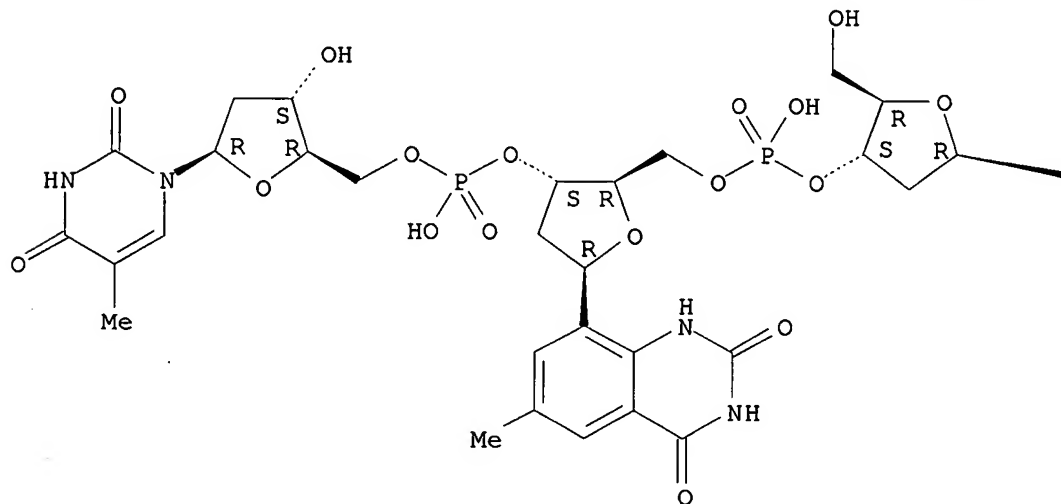
deoxyadenosine and thymidine for use in genetic system with expanded dimensions)

RN 667916-48-5 ZCAPLUS

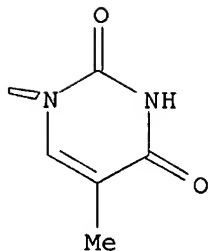
CN Thymidine, thymidylyl-(3'→5')-1'-de(6-amino-9H-purin-9-yl)-2'-deoxy-1'-(1,2,3,4-tetrahydro-6-methyl-2,4-dioxo-8-quinazolinyl)adenylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 38 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:864544 ZCAPLUS

DOCUMENT NUMBER: 140:55115

TITLE: A Four-Base Paired Genetic Helix with Expanded Size

AUTHOR(S): Liu, Haibo; Gao, Jianmin; Lynch, Stephen R.; Saito, Y. David; Maynard, Lystranne; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA

SOURCE: Science (Washington, DC, United States) (2003), 302(5646), 868-871

CODEN: SCIEAS; ISSN: 0036-8075

PUBLISHER: American Association for the Advancement of Science
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We describe a new mol. class of genetic-pairing system that has a native DNA backbone but has all four base pairs replaced by new, larger pairs. The base pairs include size-expanded analogs of thymine and of adenine, both extended by the width of a benzene ring (2.4 Å). The expanded-diameter double helixes are more thermodynamically stable than the Watson-Crick helix, likely because of enhanced base stacking. Structural data confirm a right-handed, double-stranded, and base-paired helical form. Because of the larger base size, all the pairs of this helical system are fluorescent, which suggests practical applications in detection of natural DNA and RNA. Our findings establish that there is no apparent structural or thermodyn. prohibition against genetic systems having sizes different from the natural one.

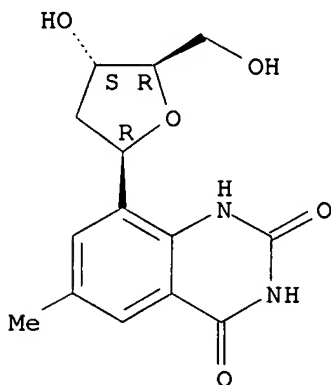
IT 639465-38-6

RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (properties of DNA analog with thymine and adenine analogs reflecting expanded size)

RN 639465-38-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-6-one, 8-(2-deoxy-β-D-erythro-pentofuranosyl)-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 39 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:841844 ZCAPLUS

DOCUMENT NUMBER: 140:77101

TITLE: The design and synthesis of novel orally active inhibitors of AP-1 and NF-κB mediated transcriptional activation. SAR of In vitro and In vivo studies

AUTHOR(S): Palanki, Moorthy S. S.; Erdman, Paul E.; Ren, Minghuan; Suto, Mark; Bennett, Brydon L.; Manning, Anthony; Ransone, Lynn; Spooner, Cheryl; Desai, Sonal; Ow, Arnie; Totsuka, Ryuichi; Tsao, Peter; Toriumi, Wataru

CORPORATE SOURCE: Celgene, San Diego, CA, 92121, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(22), 4077-4080

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:77101

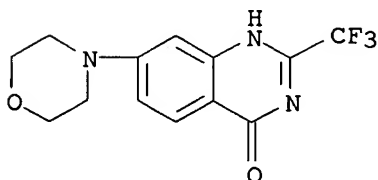
AB We have developed novel orally active quinazoline analogs as inhibitors of AP-1 and NF- κ B mediated transcriptional activation. Among the derivs. prepared, 1-[2-(2-thienyl)quinazolin-4-ylamino]-3-methyl-3-pyrroline-2,5-dione showed significant activity in an adjuvant-induced arthritis rat model by reducing the swelling by 65% in the non-injected foot. The synthesis, structure-activity relationship, and in vivo activity are described.

IT 640297-58-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and structure-activity relationships of quinazoline analogs as orally active inhibitors of AP-1 and NF- κ B mediated transcriptional activation)

RN 640297-58-1 ZCAPLUS

CN 4(1H)-Quinazolinone, 7-(4-morpholinyl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

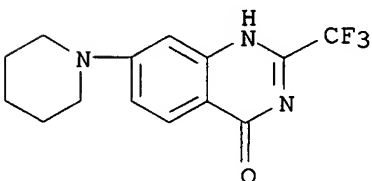


IT 219774-02-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and structure-activity relationships of quinazoline analogs as orally active inhibitors of AP-1 and NF- κ B mediated transcriptional activation)

RN 219774-02-4 ZCAPLUS

CN 4(1H)-Quinazolinone, 7-(1-piperidinyl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:737747 ZCAPLUS

DOCUMENT NUMBER: 139:261314

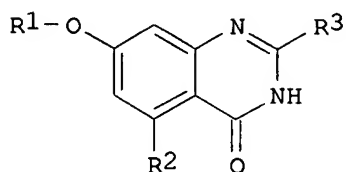
TITLE: Preparation of alkoxy quinazolinone compounds as α 1L adrenoceptors antagonists useful in therapy

INVENTOR(S): Blagg, Julian; Fray, Michael Jonathan; Lewis, Mark
 Llewellyn; Mathias, John Paul; Stefaniak, Mark Henryk;
 Stobie, Alan

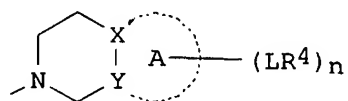
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
 SOURCE: PCT Int. Appl., 247 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076427	A1	20030918	WO 2003-IB998	20030305
WO 2003076427	A8	20041007		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2479016	A1	20030918	CA 2003-2479016	20030305
AU 2003209594	A1	20030922	AU 2003-209594	20030305
EP 1483257	A1	20041208	EP 2003-743965	20030305
EP 1483257	B1	20060913		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008407	A	20050111	BR 2003-8407	20030305
JP 2005532275	T	20051027	JP 2003-574644	20030305
AT 339414	T	20061015	AT 2003-743965	20030305
US 2004029859	A1	20040212	US 2003-387106	20030312
US 6936619	B2	20050830		
PRIORITY APPLN. INFO.:			GB 2002-6033	A 20020314
			US 2002-374894P	P 20020423
			WO 2003-IB998	W 20030305

OTHER SOURCE(S): MARPAT 139:261314
 GI



I

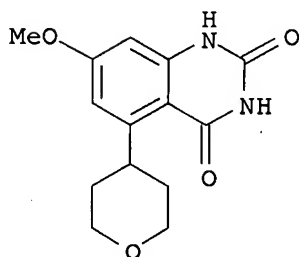


II

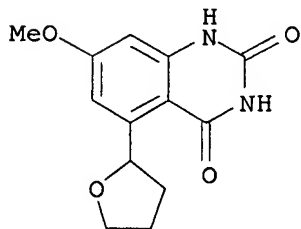
AB Quinazolinones (shown as I; variables defined below; e.g. 5-cyclopropyl-2-[5-[(cyclopropylamino)methyl]-3,4-dihydro-2(1H)-isoquinolinyl]-7-methoxy-4(3H)-quinazolinone (II)) or pharmaceutically acceptable salts or solvates thereof are useful in the treatment of hypertension, myocardial infarction, male erectile dysfunction (MED), hyperlipidemia, cardiac arrhythmia, glaucoma and benign prostatic hyperplasia (BPH). For I: R1 = C1-4 alkyl; R2 = halo, C1-4 alkyl, C3-6 cycloalkyl, C3-6 cycloalkyloxy, -SO2(C1-4 alkyl), (un)substituted C1-4 alkyloxy, Het or -OHet; R3 = bicyclic II wherein X and Y = C and N, provided that at least one is C; Ring A together with X and Y = a 5- or 6-membered aromatic, ring containing 0-3 N atoms in the ring; n is 0-2; L = a direct link, C1-4 alkylene or C1-4 alkoxyalkylene; R4 = H, -NR5R6, C3-6

cycloalkyl, -OR7, Het1 or Het4; R5 and R6 = H, C3-6 cycloalkyl, C3-6 cycloalkyl-C1-4 alkylene, -SO2(C1-4 alkyl) and (un)substituted C1-4 alkyl. R7 = H, C1-4 alkyl, C1-4 alkoxyalkyl, C3-6cycloalkyl, Het2 and C1-4alkyl-Het3; R8 is H or C1-4 alkyl; Het, Het1, Het2 and Het3 = an (un)substituted 4 to 7 membered saturated heterocyclic group which may be mono- or bi-cyclic and which contains ≥ 1 heteroatoms = N, O or S; Het4 = an (un)substituted 5 or 6 membered unsatd. heterocyclic group containing ≥ 1 heteroatoms = N, O or S; R9 = H or C1-4 alkyl; R10 and R11 = H and C1-4 alkyl. They also find utility in the treatment of female sexual arousal dysfunction (FSAD). $\alpha 1$ L adrenoceptors antagonist activity of 10 examples of I are tabulated. Three hundred seven example preps. and/or characterization data of intermediates and 133 of I are included. For example, II was prepared from N-[(1,2,3,4-tetrahydro-5-isoquinolinyl)methyl]cyclopropanamine dihydrochloride (preparation given), 2-chloro-5-cyclopropyl-7-methoxy-4(3H)-quinazolinone (preparation given) and diisopropylethylamine in butanol.

IT 601516-64-7P, 7-Methoxy-5-(tetrahydropyran-4-yl)-1H-quinazoline-2,4-dione 601516-70-5P, 7-Methoxy-5-(tetrahydrofuran-2-yl)-1H-quinazoline-2,4-dione
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of alkoxy quinazolinone compds. as $\alpha 1$ L adrenoceptors antagonists useful in therapy)
 RN 601516-64-7 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinedione, 7-methoxy-5-(tetrahydro-2H-pyran-4-yl)- (9CI)
 (CA INDEX NAME)



RN 601516-70-5 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinedione, 7-methoxy-5-(tetrahydro-2-furanyl)- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 41 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:737738 ZCAPLUS

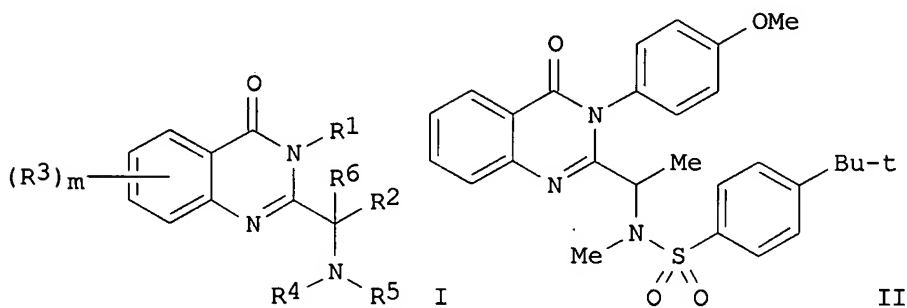
DOCUMENT NUMBER: 139:261313

TITLE: Quinazolinone amide compounds as modulators of nuclear

receptors, particularly farnesoid X receptor (FXR) and/or orphan nuclear receptors, and their preparation, pharmaceutical compositions, and methods of use

INVENTOR(S): Martin, Richard; Kahl, Jeffery Dean; Flatt, Brenton Todd; Griffith, Ronald
 PATENT ASSIGNEE(S): X-Cepto Therapeutics, Inc., USA
 SOURCE: PCT Int. Appl., 204 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076418	A1	20030918	WO 2003-US6793	20030304
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003228283	A1	20030922	AU 2003-228283	20030304
EP 1521746	A1	20050413	EP 2003-726031	20030304
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRIORITY APPLN. INFO.:			US 2002-363132P	P 20020307
			WO 2003-US6793	W 20030304
OTHER SOURCE(S):	MARPAT 139:261313			
GI				



AB Compds., pharmaceutical compns., and methods for modulating the activity of nuclear receptors are provided. In particular, amide-containing quinazolinones are provided for modulating the activity of farnesoid X receptor (FXR) and/or orphan nuclear receptors. The disclosed compds. include I [$m = 0-4$; $R^1 = H$, (un)substituted alk(en/yn)yl, (hetero)aryl, cycloalkyl(alkyl), (hetero)aralkyl, heterocycl(alkyl) (preceding groups designated as group A), OH or derivs., NH_2 or derivs.; R^2 , $R^6 =$ (independently) group A, or $R^2R^6 =$ (un)substituted alkylene; R^4 , $R^5 =$

(independently) group A, OH or derivs, NH₂ or derivs., various acyl, sulfinyl, sulfonyl, or phosphoryl groups, etc.; or R₄R₅ (un)substituted alkylene, alkenylene, alkenylene(oxy/aza)alkenylene; or any of R₂R₅, R₂R₄, R₅R₆, or R₄R₆ form 4- to 7-membered, (un)substituted heteroaryl or heterocyclyl group; R₃ = (independently) halo, pseudohalo, group A, NH₂ or derivs., OH or derivs., SH or derivs., various acyl, thioacyl, imidoyl, sulfinyl, or sulfonyl groups; or adjacent R₃R₃ = (un)substituted alkylene, alkenylene, alkylenedioxy, thioalkylenoxy, alkylenedithioxy; including stereoisomers, racemates, mixts., and pharmaceutically acceptable derivs.; with one exception compound]. Over 300 specific compds. were prepared and claimed by name. Ten of the most preferred compds. are named. The compds. are useful for treating diseases and disorders selected from: hypercholesterolemia, hyperlipoproteinemia, hypertriglyceridemia, lipodystrophy, hyperglycemia, diabetes mellitus, dyslipidemia, atherosclerosis, gallstone disease, acne vulgaris, acneiform skin conditions, diabetes, Parkinson's disease, cancer, Alzheimer's disease, inflammation, immunol. disorders, lipid disorders, obesity, conditions characterized by a perturbed epidermal barrier function, hyperlipidemia, cholestasis, peripheral occlusive disease, ischemic stroke, obesity, disease states associated with elevated cholesterol levels, conditions of disturbed differentiation or excess proliferation of the epidermis or mucous membrane, and cardiovascular disorders. For instance, Me anthranilate was N-amidated with 2-chloropropionyl chloride (97%), followed by saponification of the ester (97%), and amidation/cyclocondensation

of

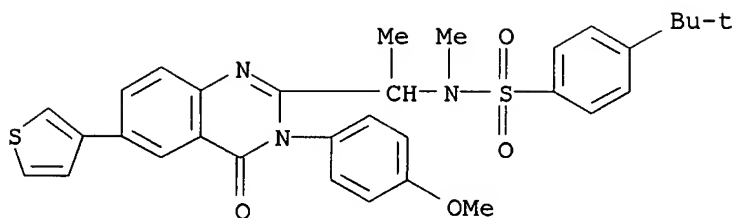
the resultant acid using p-anisidine and PCl₃ (72%), to give 2-(1-chloroethyl)-3-(4-methoxyphenyl)-3H-quinazolin-4-one. This intermediate chloride was aminated with methylamine in THF (99%), and the obtained secondary amine was sulfonylated with 4-tert-butylbenzenesulfonyl chloride and TEA in DCM (92%), to give preferred invention compound II. In an FRET assay for binding to human FXR (ligand-binding domain, fused to glutathione-S-transferase), II had an EC₅₀ of about 300 nM. In an FXR/ECREx7 co-transfection assay using African green monkey kidney cells, II had an efficacy of 190% relative to high control (chenodeoxycholic acid).

IT 602317-16-8P, 4-tert-Butyl-N-[1-[3-(4-methoxyphenyl)-4-oxo-6-(thiophen-3-yl)-3,4-dihydroquinazolin-2-yl]ethyl]-N-methylbenzenesulfonamide 602317-18-0P, 4-tert-Butyl-N-[1-[3-(4-methoxyphenyl)-4-oxo-6-(thiophen-2-yl)-3,4-dihydroquinazolin-2-yl]ethyl]-N-methylbenzenesulfonamide 602317-33-9P, 4-tert-Butyl-N-methyl-N-[1-(6-morpholin-4-yl-4-oxo-3-p-tolyl-3,4-dihydroquinazolin-2-yl)ethyl]benzenesulfonamide 602317-35-1P, 4-tert-Butyl-N-[1-[3-(4-methoxyphenyl)-4-oxo-6-pyrrolidin-1-yl-3,4-dihydroquinazolin-2-yl]ethyl]-N-methylbenzenesulfonamide 602317-37-3P, 4-tert-Butyl-N-methyl-N-[1-[4-oxo-6-(piperidin-1-yl)-3-p-tolyl-3,4-dihydroquinazolin-2-yl]ethyl]benzenesulfonamide
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinazolinone amides as farnesoid X and/or orphan nuclear receptor modulators)

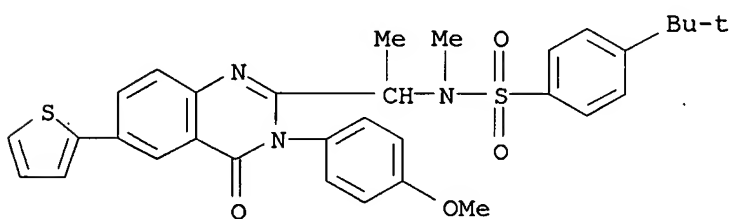
RN 602317-16-8 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3,4-dihydro-3-(4-methoxyphenyl)-4-oxo-6-(3-thienyl)-2-quinazolinyl]ethyl]-4-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)



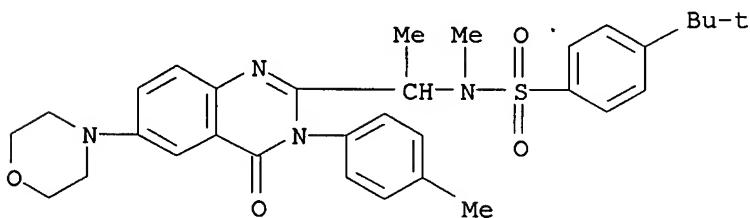
RN 602317-18-0 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3,4-dihydro-3-(4-methoxyphenyl)-4-oxo-6-(2-thienyl)-2-quinazolinyl]ethyl]-4-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)



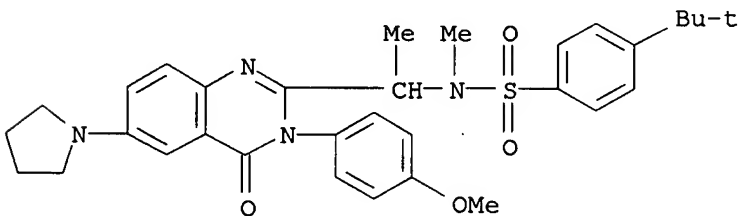
RN 602317-33-9 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3,4-dihydro-3-(4-methylphenyl)-6-(4-morpholinyl)-4-oxo-2-quinazolinyl]ethyl]-4-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 602317-35-1 ZCAPLUS

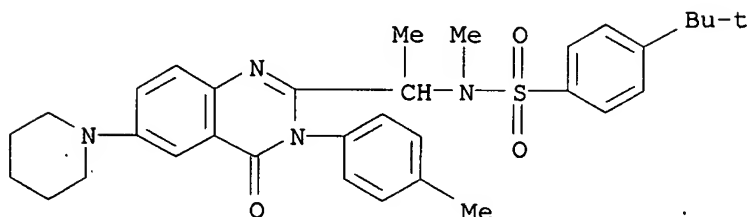
CN Benzenesulfonamide, N-[1-[3,4-dihydro-3-(4-methoxyphenyl)-4-oxo-6-(1-pyrrolidinyl)-2-quinazolinyl]ethyl]-4-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 602317-37-3 ZCAPLUS

CN Benzenesulfonamide, N-[1-[3,4-dihydro-3-(4-methylphenyl)-4-oxo-6-(1-

piperidinyl)-2-quinazolinyl]ethyl]-4-(1,1-dimethylethyl)-N-methyl- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 42 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:591156 ZCAPLUS

DOCUMENT NUMBER: 139:149640

TITLE: Preparation of substituted quinazolin-4-ylamine analogs as VR1 capsaicin receptor antagonists for relieving pain

INVENTOR(S): Bakthavatchatam, Rajagopal; Blum, Charles A.; Brielmann, Harry L.; Caldwell, Timothy M.; De Lombaert, Stephane

PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: PCT Int. Appl., 294 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

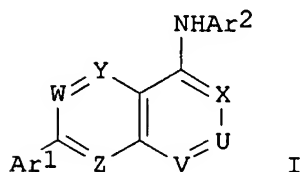
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WO 2003062209	A2	20030731	WO 2003-US1563	20030117
WO 2003062209	A3	20030904		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2473796	A1	20030731	CA 2003-2473796	20030117
BR 2003006982	A	20041026	BR 2003-6982	20030117
EP 1471910	A2	20041103	EP 2003-703887	20030117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1627944	A	20050615	CN 2003-802452	20030117
HU 200500200	A2	20050728	HU 2005-200	20030117
JP 2005526714	T	20050908	JP 2003-562090	20030117
US 2004106616	A1	20040603	US 2003-347210	20030121
US 7074799	B2	20060711		
IN 2004DN01958	A	20050401	IN 2004-DN1958	20040708
ZA 2004005641	A	20050715	ZA 2004-5641	20040715
NO 2004003411	A	20040924	NO 2004-3411	20040816

US 2006173003
PRIORITY APPLN. INFO.:

A1 20060803

US 2006-345926 20060201
US 2002-349920P P 20020117
US 2002-350527P P 20020122
WO 2003-US1563 W 20030117
US 2003-347210 A3 20030121

OTHER SOURCE(S): MARPAT 139:149640
GI



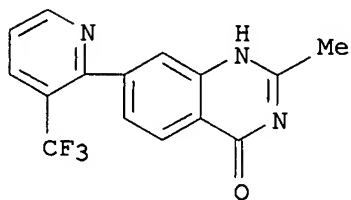
- AB Substituted quinazolin-4-ylamine analogs (shown as I; variables defined below; e.g. (4-trifluoromethylphenyl)[7-(2-trifluoromethylphenyl)quinazolin-4-yl]amine) are provided. Such compds. are ligands that may be used to modulate VR1 capsaicin receptor activity in vivo or in vitro (no data), and are particularly useful in the treatment of conditions associated with pathol. receptor activation in humans, domesticated companion animals and livestock animals. Pharmaceutical compns. and methods for using them to treat such disorders are provided, as are methods for using such ligands for receptor localization studies. For I; V, X, W, Y and Z are each independently N or CR1, with the proviso that at least one of V and X is N; U is N or CR2, with the proviso that if V and X are N, then U is CR2; R1 = H, halogen, hydroxy, amino, C1-C8 alkyl, haloC1-C8alkyl, C1-C8alkoxy, haloC1-C8alkoxy and mono- and di(C1-C8alkyl)amino. R2 = (i) H, halogen, cyano, or -COOH; (ii) C1-C8alkanoyl, C2-C8alkanone, or C1-C8carbamate, each of which is (un)substituted with 1-9 substituents = Rb, or (iii) -Rc-M-A-Ry, wherein: Rc is C0-C3alkyl; M is a bond, N(Rz), O, S, SO2, (C:O)pN(Rz), N(Rz)(C:O)p, SO2N(Rz), or N(Rz)SO2, wherein p is 0 or 1; A is a bond or C1-C8alkyl, (un)substituted with 1-3 Rb. Ry and Rz, if present, are: (a) independently H, C1-C8alkyl, C2-C8alkenyl, C2-C8alkynyl, C6-C10arylC1-C8alkyl ether, C1-C8alkoxy, a 4- to 10-membered carbocycle or heterocycle, or joined to R1 to form a 4- to 10-membered carbocycle or heterocycle, wherein each Ry and Rz = (un)substituted with 1-9 Rb; or (b) joined to form a 4- to 10-membered carbocycle or heterocycle that is (un)substituted with 1-9 Rb; Ar2 is a 5- to 7-membered aromatic heterocycle, (un)substituted with 1-3 LRa. Ar1 is a 5- to 10-membered aromatic carbocycle or heterocycle, (un)substituted with 1-3 LRa; L = bond, -O-, -C(O)-, -OC(O)-, -C(O)O-, -O-C(O)O-, -S(O)m-, -NRx-, -C(O)NHRx-, -NHRxC(O)-, -NRxS(O)m-, -S(O)mNRx- and -N[S(O)mRx]S(O)m-; wherein m = 0, 1 and 2; and Rx = H and C1-C8alkyl; Ra = (i) H, halogen, cyano and nitro; and (ii) C1-C8alkyl, C2-C8alkenyl, C2-C8alkynyl, C2-C8alkyl ether, 3- to 10-membered heterocycles, mono- and di(C1-C8alkyl)amino and (3- to 10-membered heterocycle)C1-C6 alkyl, each of which is (un)substituted with 1-9 Rb. Rb = hydroxy, halogen, amino, aminocarbonyl, amido, cyano, nitro, C1-C8alkyl, C1-C8alkoxy, C1-C8alkylthio, C1-C8alkyl ether, hydroxyC1-C8alkyl, haloC1-C8alkyl, Ph, phenyl(C1-C8alkyl), mono and di(C1-C6 alkyl)amino, (SO2)C1-C8alkyl, 5- to 7-membered heterocycle and (5- to 7-membered heterocycle)(C1-C8alkyl). Although the methods of preparation are not claimed, many example preps. and characterization data for >500 examples of I are included.
- IT 573675-91-9P, 2-Methyl-7-(3-trifluoromethylpyridin-2-yl)quinazolin-4-ol 573680-42-9P, 2-Chloromethyl-7-(3-trifluoromethylpyridin-2-yl)-3H-quinazolin-4-one 573680-86-1P, 2-[2-(Benzyloxy)ethyl]-7-(3-trifluoromethylpyridin-2-yl)-3H-quinazolin-4-one 573681-00-2P

, 3-[4-Hydroxy-7-(3-trifluoromethylpyridin-2-yl)quinazolin-2-yl]propionic acid ethyl ester 573686-47-2P, 2-(2-Methoxyethyl)-7-(3-trifluoromethylpyridin-2-yl)quinazolin-4-ol 573686-50-7P, 2-[3-(Benzyloxy)propyl]-7-(3-trifluoromethylpyridin-2-yl)quinazolin-4-ol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted quinazolin-4-ylamine analogs as VR1 capsaicin receptor antagonists for relieving pain and for detecting receptors)

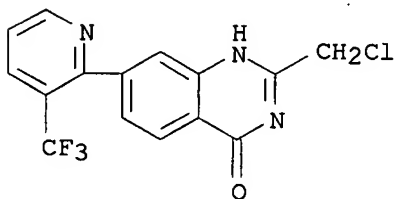
RN 573675-91-9 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-methyl-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI)
 (CA INDEX NAME)



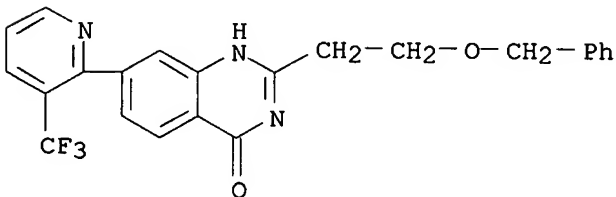
RN 573680-42-9 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-(chloromethyl)-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



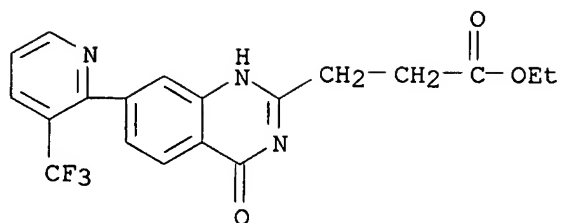
RN 573680-86-1 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[2-(phenylmethoxy)ethyl]-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



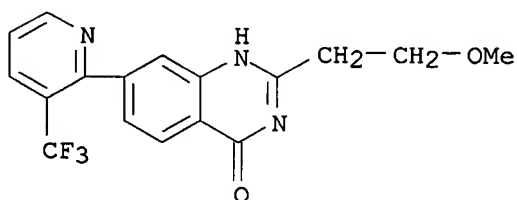
RN 573681-00-2 ZCAPLUS

CN 2-Quinazolinepropanoic acid, 1,4-dihydro-4-oxo-7-[3-(trifluoromethyl)-2-pyridinyl]-, ethyl ester (9CI) (CA INDEX NAME)



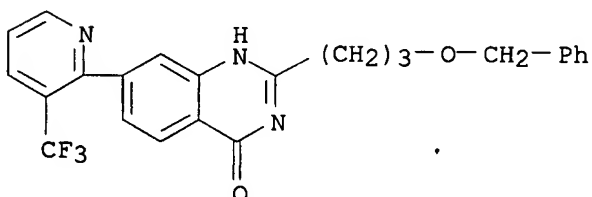
RN 573686-47-2 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-(2-methoxyethyl)-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 573686-50-7 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[3-(phenylmethoxy)propyl]-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 43 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:511320 ZCAPLUS

DOCUMENT NUMBER: 139:85370

TITLE: Preparation of quinazolinone derivatives as inosine 5'-monophosphate dehydrogenase (IMPDH) inhibitors for use in pharmaceutical compositions

INVENTOR(S): Dyke, Hazel Joan; Richard, Marianna Dilani; Haughan, Alan Findlay; Sharpe, Andrew

PATENT ASSIGNEE(S): Celltech R & D Limited, UK

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053958	A1	20030703	WO 2002-GB5770	20021218
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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AU 2002352444

A1 20030709

AU 2002-352444

20021218

PRIORITY APPLN. INFO.:

GB 2001-30585

A 20011220

GB 2002-4137

A 20020222

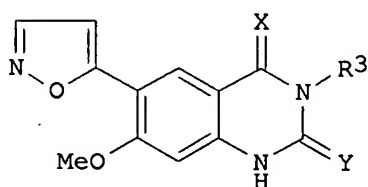
WO 2002-GB5770

W 20021218

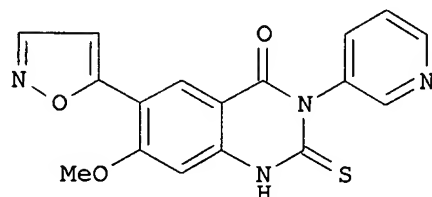
OTHER SOURCE(S):

MARPAT 139:85370

GI



I



II

AB Quinazolinones, such as I [X, Y = O, S; R₃ = alkyl, heterocyclyl, heterocyclylalkyl, aminoalkyl, etc.], were prepared for therapeutic use as IMPDH inhibitors for therapeutic use in the treatment of cancer, inflammatory disorders, autoimmune disorders, psoriatic disorders and viral disorders. Thus, quinazolinone derivative II was prepared via a cyclocondensation reaction of 2-isothiocyanato-4-methoxy-5-(5-oxazolyl)benzoic acid Me ester with 3-aminopyridine. The prepared quinazolinones were assayed for inhibition of IMPDH and for inhibition of human peripheral blood mononuclear cells.

IT 553678-60-7P 553678-71-0P 553678-74-3P

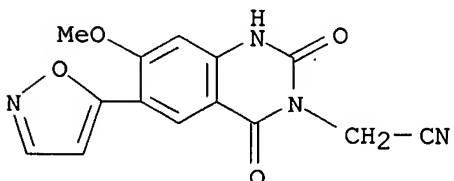
553679-12-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of quinazolinone derivs. as IMPDH inhibitors for use in pharmaceutical compns.)

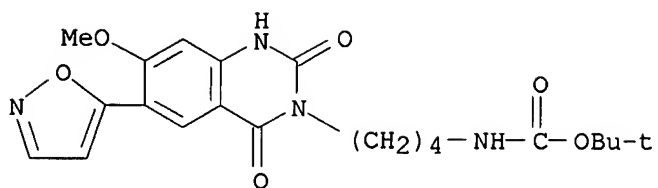
RN 553678-60-7 ZCAPLUS

CN 3(2H)-Quinazolineacetonitrile, 1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo- (9CI) (CA INDEX NAME)



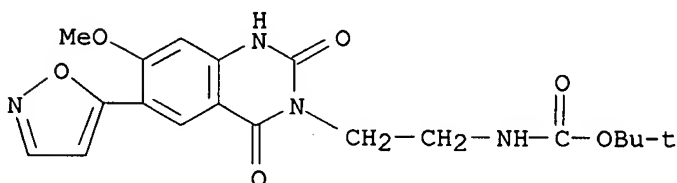
RN 553678-71-0 ZCAPLUS

CN Carbamic acid, [4-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



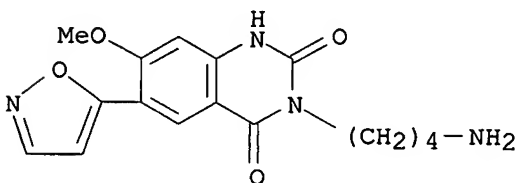
RN 553678-74-3 ZCAPLUS

CN Carbamic acid, [2-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 553679-12-2 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-(4-aminobutyl)-6-(5-isoxazolyl)-7-methoxy-(9CI) (CA INDEX NAME)



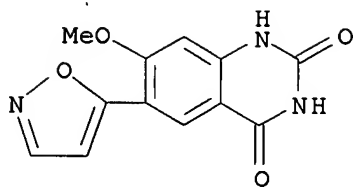
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 553678-54-9P 553678-56-1P 553678-58-3P
 553678-62-9P 553678-65-2P 553678-68-5P
 553678-75-4P 553678-76-5P 553678-78-7P
 553678-81-2P 553678-83-4P 553678-85-6P
 553678-87-8P 553678-89-0P 553678-91-4P
 553678-94-7P 553678-96-9P 553678-98-1P
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 553679-07-5P 553679-09-7P 553679-11-1P
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 553679-16-6P 553679-17-7P 553679-18-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazolinedione derivs. as IMPDH inhibitors for use in pharmaceutical compns.)

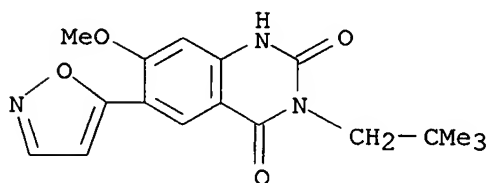
RN 553678-43-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



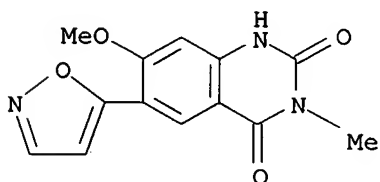
RN 553678-45-8 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-(2,2-dimethylpropyl)-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



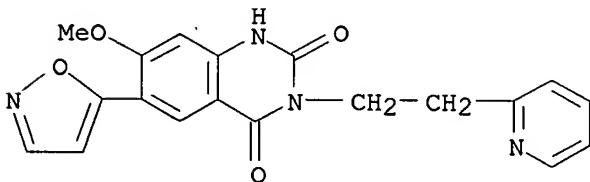
RN 553678-46-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-methyl- (9CI) (CA INDEX NAME)



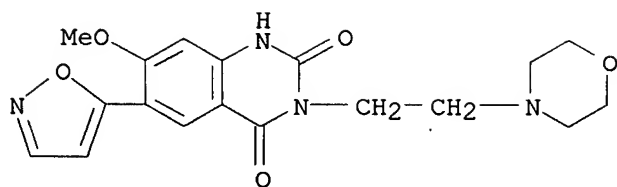
RN 553678-48-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



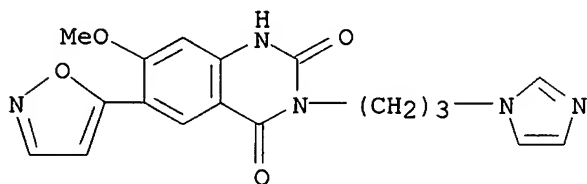
RN 553678-50-5 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)



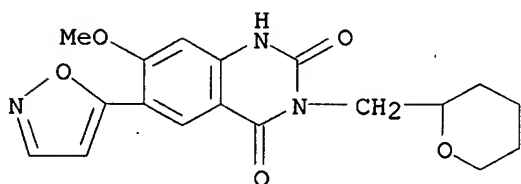
RN 553678-52-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-[3-(1H-imidazol-1-yl)propyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



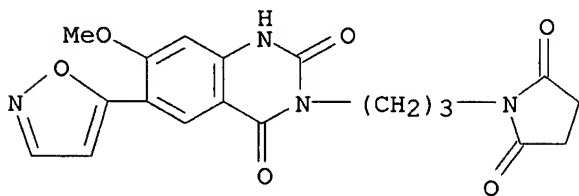
RN 553678-54-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[(tetrahydro-2H-pyran-2-yl)methyl]- (9CI) (CA INDEX NAME)



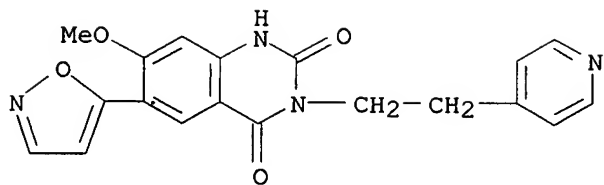
RN 553678-56-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



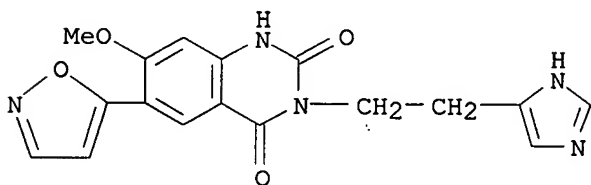
RN 553678-58-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



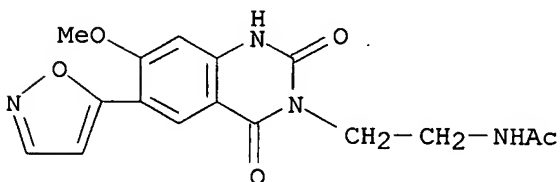
RN 553678-62-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-[2-(1H-imidazol-4-yl)ethyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



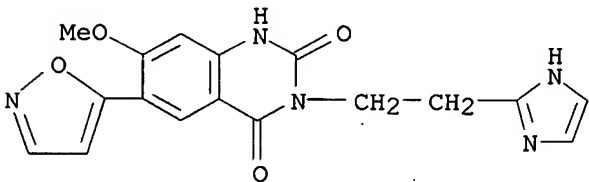
RN 553678-65-2 ZCAPLUS

CN Acetamide, N-[2-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]ethyl]- (9CI) (CA INDEX NAME)



RN 553678-68-5 ZCAPLUS

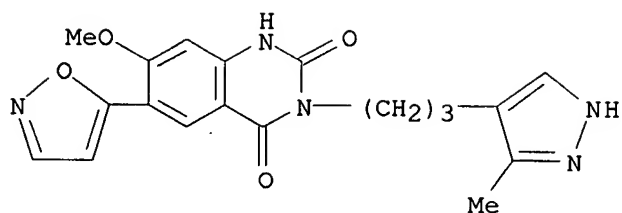
CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-[2-(1H-imidazol-2-yl)ethyl]-6-(5-isoxazolyl)-7-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

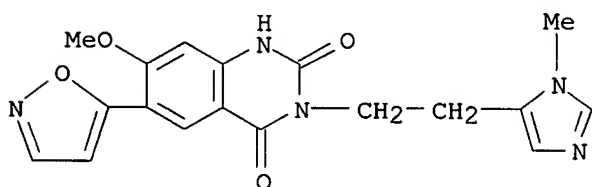
RN 553678-75-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[3-(3-methyl-1H-pyrazol-4-yl)propyl]- (9CI) (CA INDEX NAME)



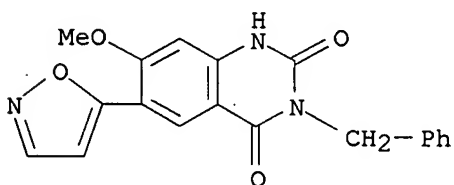
RN 553678-76-5 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-[2-(1-methyl-1H-imidazol-5-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 553678-78-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



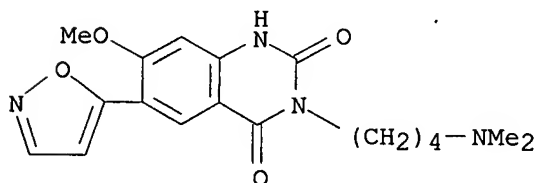
RN 553678-81-2 ZCAPLUS

CN Formic acid, compd. with 3-[4-(dimethylamino)butyl]-6-(5-isoxazolyl)-7-methoxy-2,4(1H,3H)-quinazolinedione (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 553678-80-1

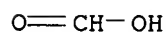
CMF C18 H22 N4 O4



CM 2

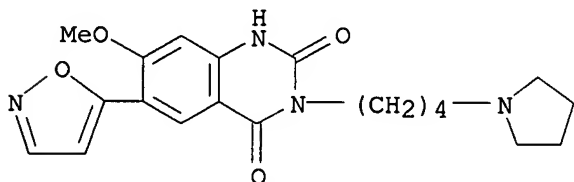
CRN 64-18-6

CMF C H2 O2



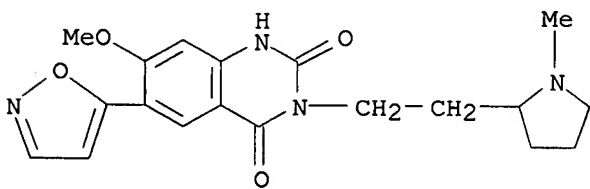
RN 553678-83-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-[4-(1-pyrrolidiny)butyl]- (9CI) (CA INDEX NAME)



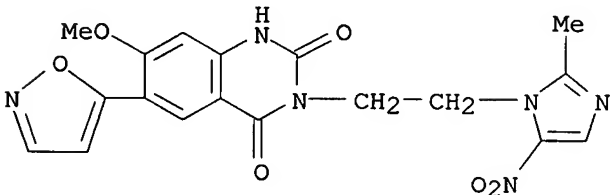
RN 553678-85-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-[2-(1-methyl-2-pyrrolidiny)ethyl]- (9CI) (CA INDEX NAME)



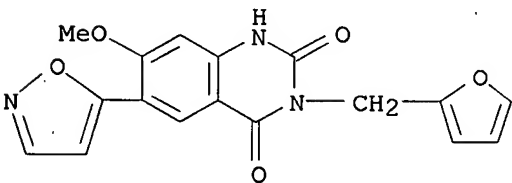
RN 553678-87-8 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-[2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 553678-89-0 ZCAPLUS

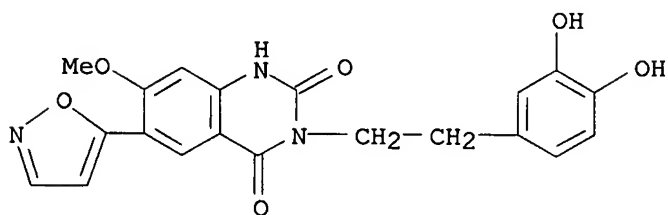
CN 2,4(1H,3H)-Quinazolinedione, 3-(2-furanylmethyl)-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



10/ 530,897

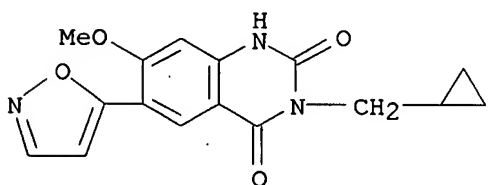
RN 553678-91-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-[2-(3,4-dihydroxyphenyl)ethyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



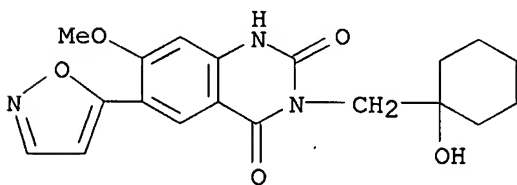
RN 553678-94-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-(cyclopropylmethyl)-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



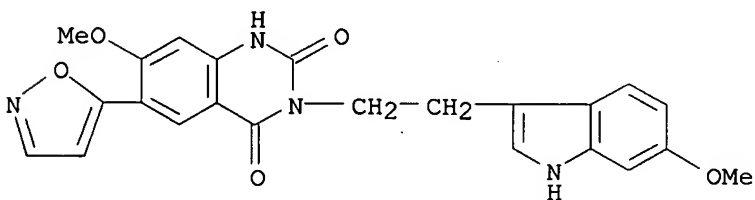
RN 553678-96-9 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-[(1-hydroxycyclohexyl)methyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



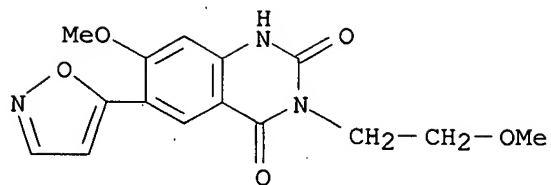
RN 553678-98-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-[2-(6-methoxy-1H-indol-3-yl)ethyl]- (9CI) (CA INDEX NAME)



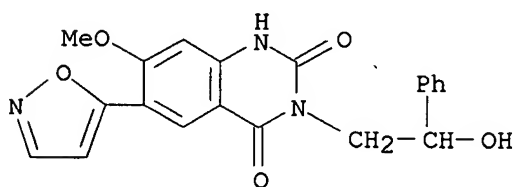
RN 553679-00-8 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(5-isoxazolyl)-7-methoxy-3-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



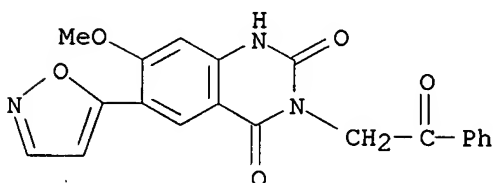
RN 553679-02-0 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-(2-hydroxy-2-phenylethyl)-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



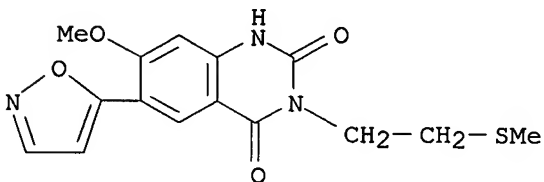
RN 553679-05-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)



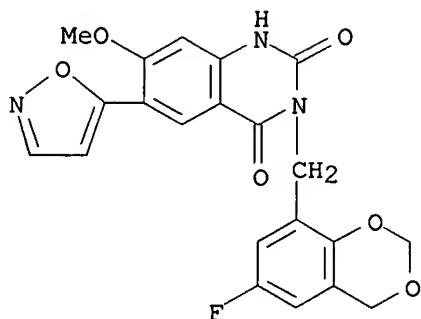
RN 553679-07-5 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 6-(5-isoxazolyl)-7-methoxy-3-[2-(methylthio)ethyl]- (9CI) (CA INDEX NAME)



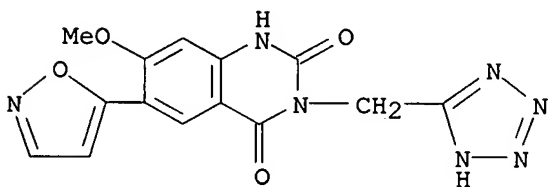
RN 553679-09-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2(1H)-one, 3-[(6-fluoro-4H-1,3-benzodioxin-8-yl)methyl]-6-(5-isoxazolyl)-7-methoxy- (9CI) (CA INDEX NAME)



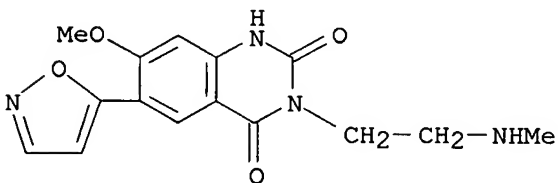
RN 553679-11-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 6-(5-isoxazolyl)-7-methoxy-3-(1H-tetrazol-5-ylmethyl)- (9CI) (CA INDEX NAME)



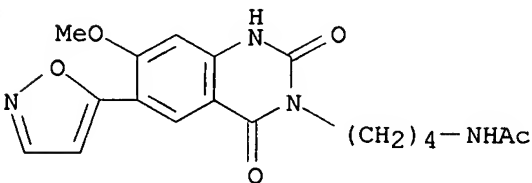
RN 553679-13-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolin-2-one, 6-(5-isoxazolyl)-7-methoxy-3-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



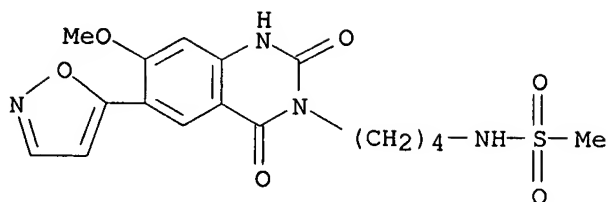
RN 553679-14-4 ZCAPLUS

CN Acetamide, N-[4-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]butyl]- (9CI) (CA INDEX NAME)



RN 553679-15-5 ZCAPLUS

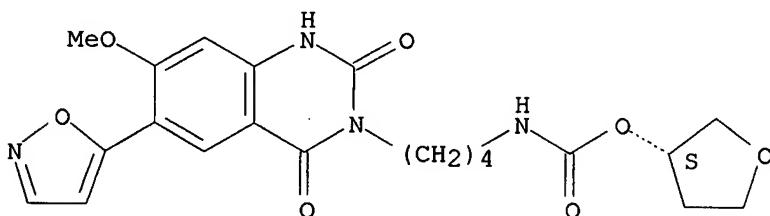
CN Methanesulfonamide, N-[4-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]butyl]- (9CI) (CA INDEX NAME)



RN 553679-16-6 ZCAPLUS

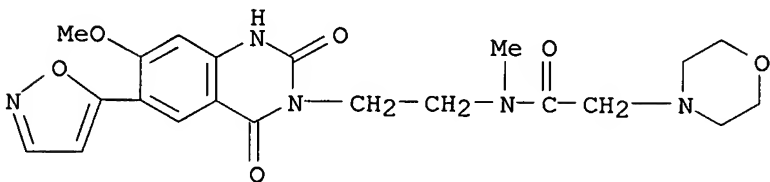
CN Carbamic acid, [4-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]butyl]-, (3S)-tetrahydro-3-furanyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



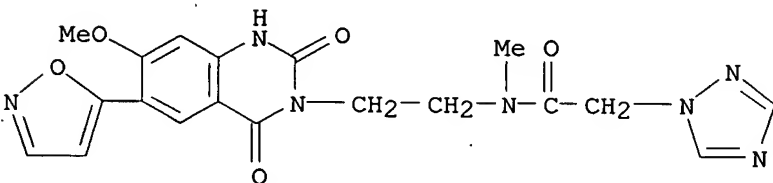
RN 553679-17-7 ZCAPLUS

CN 4-Morpholineacetamide, N-[2-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]ethyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 553679-18-8 ZCAPLUS

CN 1H-1,2,4-Triazole-1-acetamide, N-[2-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]ethyl]-N-methyl- (9CI) (CA INDEX NAME)



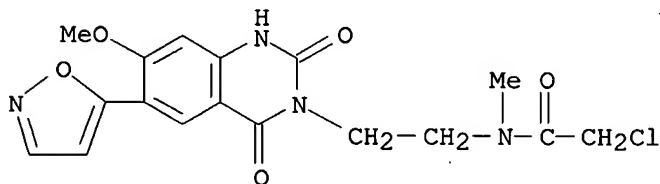
IT 553678-01-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinazolinone derivs. as IMPDH inhibitors for use in pharmaceutical comps.)

RN 553678-01-6 ZCAPLUS

CN Acetamide, 2-chloro-N-[2-[1,4-dihydro-6-(5-isoxazolyl)-7-methoxy-2,4-dioxo-3(2H)-quinazolinyl]ethyl]-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 44 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:524036 ZCAPLUS

DOCUMENT NUMBER: 137:232614

TITLE: A Traceless Approach for the Parallel Solid-Phase Synthesis of 2-(Arylamino)quinazolinones

AUTHOR(S): Yu, Yongping; Ostresh, John M.; Houghten, Richard A.

CORPORATE SOURCE: Torrey Pines Institute for Molecular Studies, San Diego, CA, 92121, USA

SOURCE: Journal of Organic Chemistry (2002), 67(16), 5831-5834
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:232614

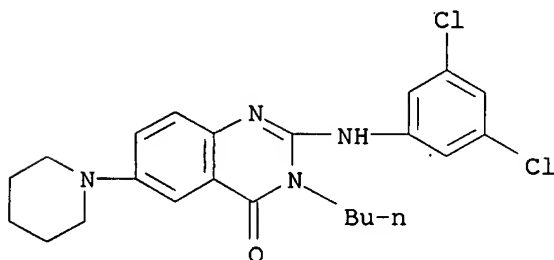
AB A traceless approach for the parallel solid-phase synthesis of 2-arylamino-substituted quinazolinones is described. Acylation of MBHA resin with o-nitrobenzoic acid derivs., followed by reduction of the nitro group with tin chloride, generated a resin-bound o-anilino derivative. Reaction of resin-bound o-anilino derivative with aryl isothiocyanates yielded resin-bound thioureas, which reacted with amines in the presence of Mukaiyama's reagent (2-chloro-1-methylpyridinium iodide) to afford resin-bound guanidines. Following intramol. cyclization of the resin-bound guanidines during cleavage from the resin by HF/anisole (95/5) for 1.5 h at 0 °C, the desired products were obtained in good yield and purity.

IT 457887-37-5P 457887-38-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(traceless parallel solid-phase synthesis of 2-(arylamino)quinazolinones)

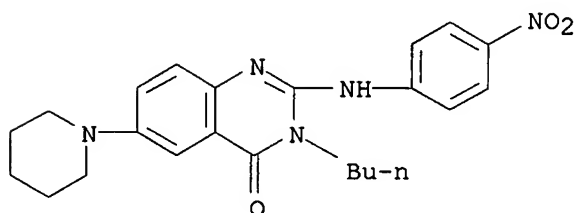
RN 457887-37-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 3-butyl-2-[(3,5-dichlorophenyl)amino]-6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



10/ 530,897

RN 457887-38-6 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-butyl-2-[(4-nitrophenyl)amino]-6-(1-piperidinyl)-
(9CI) (CA INDEX NAME)

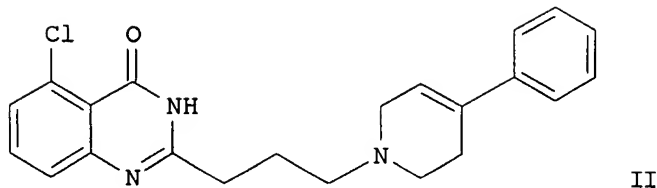
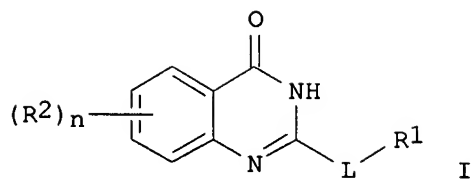


REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 45 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:465983 ZCAPLUS
DOCUMENT NUMBER: 137:47214
TITLE: Preparation of 2-substituted-4(3H)-quinazolinone
derivatives as PARP inhibitors
INVENTOR(S): Matsuoka, Nobuya; Iwashita, Akinori; Yamazaki, Shunji;
Miyake, Hiroshi; Ohkubo, Mitsuru; Kamijo, Kazunori;
Nakanishi, Isao; Hattori, Kouji; Kido, Yoshiyuki;
Ishida, Junya; Yamamoto, Hirofumi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048117	A1	20020620	WO 2001-JP10601	20011205
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2431406	A1	20020620	CA 2001-2431406	20011205
AU 2002021047	A5	20020624	AU 2002-21047	20011205
EP 1355888	A1	20031029	EP 2001-270531	20011205
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004515544	T	20040527	JP 2002-549648	20011205
US 2004077667	A1	20040422	US 2003-433947	20030609
PRIORITY APPLN. INFO.:			AU 2000-2016	A 20001211
			WO 2001-JP10601	W 20011205

OTHER SOURCE(S): MARPAT 137:47214
GI



AB Title compds. I [R^1 = (un)substituted cyclic amino group(s); R^2 = substituent; $n = 0-4$; L = alkylene, alkenylene] were prepared. For instance, 2-amino-6-chlorobenzamide was coupled to 4-pentenoyl chloride (THF, i -PrNEt₂, 5°C, 30 min) and the product treated with 1N NaOH to afford 2-(3-butenyl)-5-chloro-4(3H)-quinazolinone. This intermediate was oxidatively cleaved (dioxane, OsO₄, t -BuOH; NaIO₄) effecting cyclization to 8-chloro-1-hydroxy-2,3-dihydropyrrolo[2,1-b]quinazoline-9(1H)-one isolated as a colorless powder. This was used to alkylate 1,2,3,6-tetrahydro-4-phenylpyridine (CH₃CNaq, HOAc, NaCNBH₃) to afford II. Selected compds. of the invention had IC₅₀ < 0.5 μ M for poly(ADP-ribose)polymerase (PARP). I are useful for the treatment of NMDA- and NO-induced toxicity, tissue damage resulting from apoptosis, etc.

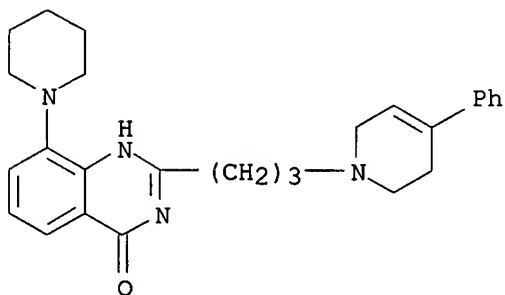
IT 437996-76-4P 437996-77-5P 437996-78-6P
437996-79-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; preparation of 2-[ω -substituted(hetero)aryl-alkyl]substituted-4(3H)-quinazolinone derivs.)

RN 437996-76-4 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[3-(3,6-dihydro-4-phenyl-1(2H)-pyridinyl)propyl]-8-(1-piperidinyl)- (9CI) (CA INDEX NAME)

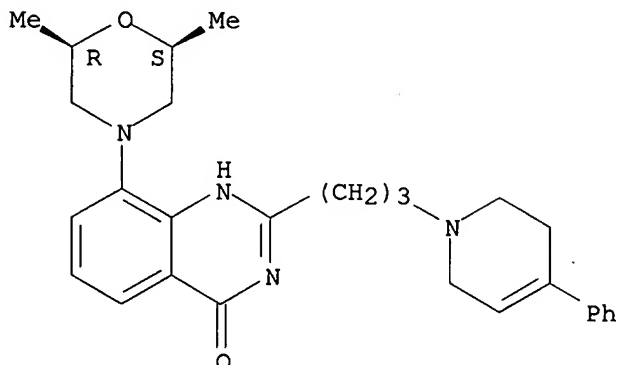


RN 437996-77-5 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[3-(3,6-dihydro-4-phenyl-1(2H)-pyridinyl)propyl]-8-

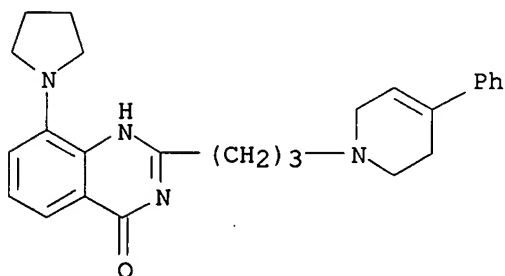
[(2R,6S)-2,6-dimethyl-4-morpholinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



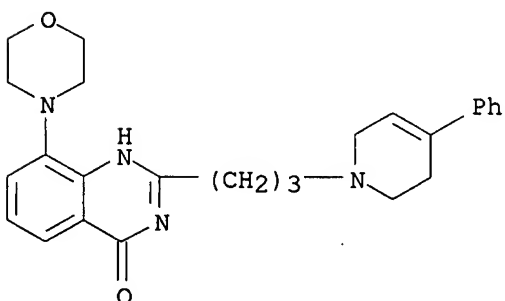
RN 437996-78-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[3-(3,6-dihydro-4-phenyl-1(2H)-pyridinyl)propyl]-8-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 437996-79-7 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-[3-(3,6-dihydro-4-phenyl-1(2H)-pyridinyl)propyl]-8-(4-morpholinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 46 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:453051 ZCAPLUS

DOCUMENT NUMBER: 135:61347

TITLE: Phthalimidoalkylquinazolinones as

phosphodiesterase-V inhibitors
 INVENTOR(S): Aletru, Michel; Bovy, Philippe R.; Namane, Claudie
 PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.
 SOURCE: PCT Int. Appl., 31 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

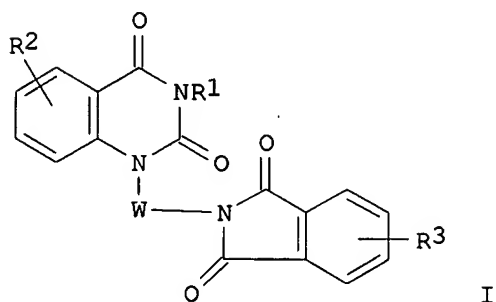
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044228	A2	20010621	WO 2000-FR3534	20001214
WO 2001044228	A3	20011213		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: FR 1999-15717 A 19991214

OTHER SOURCE(S): MARPAT 135:61347

GI



AB Title compds. I [R1 = alkyl, alkenyl, cycloalkyl, hydroxyalkyl, alkoxyalkyl; R2 = amino, aminoalkoxy, carbamoylalkoxy, alkoxy-carbonylalkoxy, nitrogen heterocyclalkoxy; R3 = H, OH, halogen, CN, NO2, amino, alkyl; W = alkylene, alkenylene] and their salts and hydrates were prepared for use as PDE-V inhibitors with IC50 <50 nM. Thus, 5-hydroxyanthranilic acid was converted to its Me ester, attached to Wang resin, treated with Me2CHNCO to give the urea, which was treated with N-bromomethylphthalimide, cleaved from the resin, and treated with BrCH2CO2CMe3 and cyclopentylamine to give I [R1 = CHMe2, R2 = 6-cyclopentylcarbamoylmethoxy, R3 = H, W = CH2].

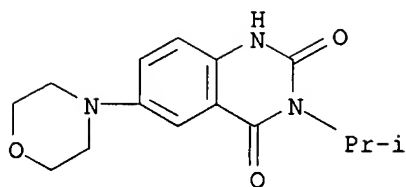
IT 345226-64-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phthalimidoalkylquinazolinones as phosphodiesterase-V inhibitors)

RN 345226-64-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinone, 3-(1-methylethyl)-6-(4-morpholinyl)- (9CI)
 (CA INDEX NAME)



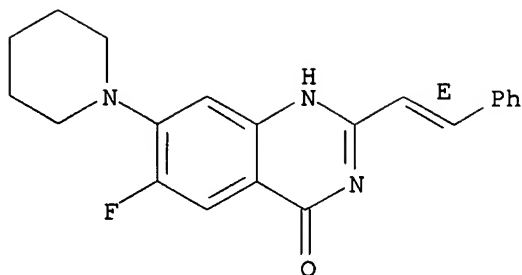
L4 ANSWER 47 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:438306 ZCAPLUS
 DOCUMENT NUMBER: 136:210029
 TITLE: Evaluation of quinolone derivatives for antitrypanosomal activity
 AUTHOR(S): Keiser, J.; Burri, C.
 CORPORATE SOURCE: Department of Medical Parasitology and Infection Biology, Swiss Tropical Institute, Basel, 4002, Switz.
 SOURCE: Tropical Medicine & International Health (2001), 6(5), 369-389
 CODEN: TMIHFL; ISSN: 1360-2276
 PUBLISHER: Blackwell Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB About 160 fluoroquinolones and derivs. were tested for antitrypanosomal activity in a drug sensitivity assay followed by fluorometric evaluation. The most active quinolone compds. had IC50 values in the range from 100 to 900 ng/mL, while several derivs. were not active at a concentration of 100 µg/mL. In a structure-activity relationship study, modification of the quinolones at position R1, R2, R3 and R8 did not influence trypanocidal activity. An exchange of the fluorine at position 6 may contribute to an increase in activity but does not entirely control it. Pyrrolidine substituents at position R7 generally were more active than other substituents at this position. Tetracyclic quinolone derivs. were amongst the most active compds. with IC50 values in the range of 0.3-8.8 µg/mL. The in vitro cytotoxicity on HT-29 cells was determined for active compds. with IC50 values below 1 µg/mL. In addition, six drugs with an IC50 below 1 µg/mL and a selectivity index of more than 10 were chosen for in vivo expts. Dose escalation expts. with a maximum dose of 100 mg/kg/bid were performed in a mouse model without central nervous system involvement. For unknown reasons the in vitro effect of the drugs could not be confirmed in vivo, but the class of compound remains of interest for their mode of action, the low toxicity, pharmacol. properties and the availability of a large number of synthesized compds.

IT 127033-43-6
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
 (antitrypanosomal activity of quinolone derivs. as function of their structure)

RN 127033-43-6 ZCAPLUS
 CN 4(1H)-Quinazolinone, 6-fluoro-2-[(1E)-2-phenylethenyl]-7-(1-piperidinyl)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 48 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:228868 ZCAPLUS

DOCUMENT NUMBER: 134:252356

TITLE: Preparation of 2-(arylamino)-4-quinazolinols as inhibitors of cleavage of protein substrates by caspase-3

INVENTOR(S): Jacobs, Robert Toms; Folmer, James; Simpson, Thomas Richard; Chaudhari, Bipinchandra; Frazee, William Jackson; Davenport, Timothy Wayne

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

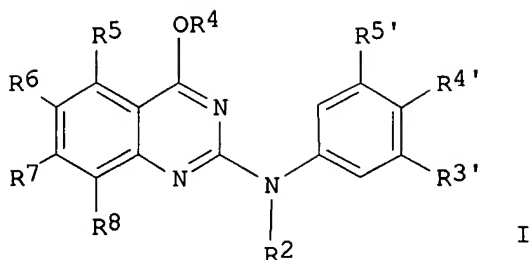
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001021598	A1	20010329	WO 2000-GB3555	20000918
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1218358	A1	20020703	EP 2000-958907	20000918
EP 1218358	B1	20060913		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
JP 2003509501	T	20030311	JP 2001-524977	20000918
AT 339406	T	20061015	AT 2000-958907	20000918
US 6399603	B1	20020604	US 2000-668322	20000922
PRIORITY APPLN. INFO.:			US 1999-155623P	P 19990923
			WO 2000-GB3555	W 20000918

OTHER SOURCE(S): MARPAT 134:252356

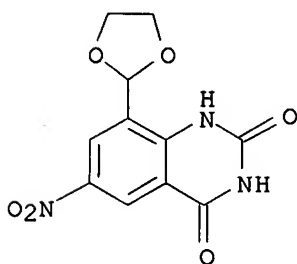
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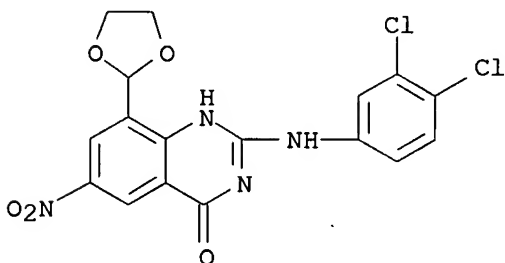
AB I (e.g. [2-[(3,4-dichlorophenyl)amino]-4-hydroxy-6-nitroquinazolin-8-yl]-N-[(4-fluorophenyl)methyl]carboxamide) or a pharmaceutically-acceptable salt thereof and methods of using such compds. for the treatment of various diseases and pharmaceutical compns. comprising such compds. are claimed. In I, R2 is H, acetyl or (C1-C5)alkyl. R4 is H, acetyl or (C1-C5)alkyl. R5, R6 and R7 are independently H, halogen, (C1-C2)alkyl, halo(C1-C2)alkyl, nitro and cyano. R8 is H, Ph, (C1-C6)alkyl, Ri, heterocycle, substituted heterocycle, -(CH2)mC(O)N-[(CH2)pRg]Rb, -(CH2)mN[(CH2)pRg]Rb, -CH:CHRC, halogen, -(CH2)mC(O)(CH2)mRo, -C(O)Rp, -(CH2)mC(O)O[(CH2)pRg], -(CH2)mN[(CH2)pRg]C(O)Rb, -(CH2)mOC(O)[(CH2)pRg], -CHORdORe, -CH2XRf, -S(O)2N[(CH2)pRg]Rb, -N[(CH2)pRg]S(O)2Rb, -S(O)2N[(CH2)pRg]Rb, -C(O)H, allyl and 4-hydroxybut-1-en-4-yl. R3', R4' and R5' are independently H, halogen, (C1-C4)alkyl, (C1-C4)alkoxy and halo(C1-C4)alkyl; wherein at least one of R5, R6, R7, R8, R3' and R5' is not H; and R4' is not equal to R7. Rb is H, (C1-C4)alkyl or substituted (C1-C4)alkyl. Rc is H, Ph, Ri, heterocycle, substituted heterocycle, -CO2Rb, -C(O)NRbRb, -S(O)n-Rf, 2-hydroxyisopropyl and cyano. Rd and Re are independently (C1-C4)alkyl; or Rd and Re together are -CH2CH2- or -CH2CH2CH2-. Rf is (C1-C4)alkyl, vinyl, -CH2CO2Rb, Ph or benzyl. Rg is (C1-C10)alkyl, substituted (C1-C10)alkyl, Ph, Ri, heterocycle, substituted heterocycle, -ORb, -NRbRb, -NRjRo, -N(Rj)SO2Rj, -CO2Rb, -C(O)NRjRj, -SO2phenyl and 2-oxopyrrolidin-1-yl; or Rg and Rb together form -CH2CH2N(Rj)CH2CH2-, -(CH2)4-, -CH(Rh)CH2CH2CH2-, or -CH2CH2OCH2CH2-. Rh is -CO2Rf or -CH2O-Ph. Ri is Ph, containing 1-3 substituents selected from halogen, (C1-C6)alkyl, -ORj, -O(substituted phenyl)-NRjRj, halo(C1-C6)alkyl, halo(C1-C4)alkoxy, nitro, -C(O)Rj, -C(O)(substituted phenyl), -(CH2)mC(O)NRjRk, -(CH2)mC(O)N(Rj)SO2[(C1-C6)alkyl], -(CH2)mC(O)NRj(substituted phenyl), -(CH2)nCO2Rj, -OC(O)Rj, -N(Rj)C(O)Rj, -NRjC(O)halo(C1-C4)alkoxy, -C(O)NRjRj, -NRjS(O)2(C1-C4)alkyl, -SON(C1-C6)alkyl, -SON(halogen), -SOM(CH2)nphenyl, -SO2NRjRj, -SO2NRjRk, -SO2NRj(substituted (C1-C6)alkyl), -SO2(CH2)nRo, -SO2N(Rj)(CH2)nRo, -SON(halo(C1-C3)alkyl), -SON(pyrrolidin-1-yl substituted in the 2 position by Rn), -CN, -SCN, Ph, heterocycle and benzyl. Rj is H or (C1-C6)alkyl. Rk is -(CH2)nCH2OCH2Rb, -C(O)NRjRj or -C(O)Rj. Rm is heterocycle, containing one or two substituents selected from halogen, (C1-C6)alkyl, -ORj, -O(substituted phenyl)-NRjRj, halo(C1-C6)alkyl, halo(C1-C4)alkoxy, nitro, -C(O)Rj, -C(O)(substituted phenyl), -(CH2)mC(O)NRjRk, -(CH2)mC(O)N(Rj)SO2[(C1-C6)alkyl], -(CH2)mC(O)NRj(substituted phenyl), -(CH2)nCO2Rj, -OC(O)Rj, -N(Ri)C(O)Rj, -NRjC(O)-halo(C1-C4)alkoxy, -C(O)NRjRj, -NRjS(O)2(C1-C4)alkyl, -SON(C1-C6)alkyl, -SON(halogen), -SOM(CH2)nphenyl, -SO2NRjRj, -SO2NRjRk, -SO2NRj(substituted (C1-C6)alkyl), -SO2(CH2)nRo, -SO2N(Rj)(CH2)nRo, -SON(halo(C1-C3)alkyl), -SON(pyrrolidin-1-yl substituted in the 2 position by Rn), -CN, -SCN, Ph, heterocycle and benzyl. Rn is -C(O)Rj, -CH2ORj or -C(O)NRjRj. Ro is Ph, substituted Ph, heterocycle or substituted heterocycle. Rp is a heterocycle containing one or two substituents selected from substituted Ph, heterocycle, Ph, benzyl, -SONRo or SO2NRjRj. M is 0-3; n is 0-2; p is 0-7; X is S, O or N. A method is claimed of treating a mammalian disease

selected from cell apoptosis, immune deficiency syndromes, autoimmune diseases, pathogenic infections, cardiovascular and neurol. injury, alopecia, aging, cancer, Parkinson's disease, Alzheimer's disease, Huntington's disease, acute and chronic neurodegenerative disorders, stroke, vascular dementia, head trauma, ALS, neuromuscular disease, myocardial ischemia, cardiomyopathy, macular degeneration, osteoarthritis, diabetes, acute liver failure and spinal cord injury. Although caspase-3 inhibition and apoptosis assay methods are described, quant. assay results are not given. Although the methods of preparation are not claimed, 17 example preps. are included.

IT 331647-23-5P, 8-(1,3-Dioxolan-2-yl)-6-nitroquinazoline-2,4-diol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of 2-(arylamino)-4-quinazolinols as inhibitors of cleavage of protein substrates by caspase-3)
 RN 331647-23-5 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinone, 8-(1,3-dioxolan-2-yl)-6-nitro- (9CI) (CA INDEX NAME)



IT 331642-50-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 2-(arylamino)-4-quinazolinols as inhibitors of cleavage of protein substrates by caspase-3)
 RN 331642-50-3 ZCAPLUS
 CN 4(1H)-Quinazolinone, 2-[(3,4-dichlorophenyl)amino]-8-(1,3-dioxolan-2-yl)-6-nitro- (9CI) (CA INDEX NAME)



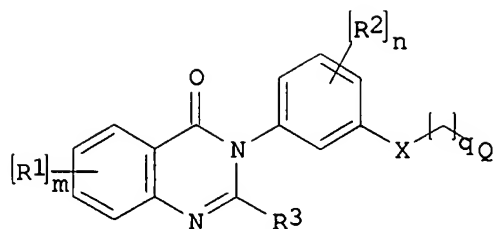
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 49 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:666727 ZCAPLUS
 DOCUMENT NUMBER: 133:252450
 TITLE: Preparation of 3-(3-amidophenyl)-3,4-dihydroquinazolin-4-ones for treating diseases mediated by cytokines

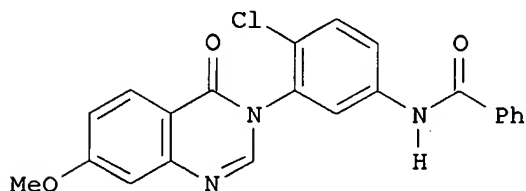
INVENTOR(S): Brown, Dearg Sutherland
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 145 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055153	A1	20000921	WO 2000-GB912	20000313
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2368097	A1	20000921	CA 2000-2368097	20000313
EP 1163237	A1	20011219	EP 2000-909498	20000313
EP 1163237	B1	20040506		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000009083	A	20020102	BR 2000-9083	20000313
TR 200103336	T2	20020422	TR 2001-3336	20000313
HU 200105114	A2	20020729	HU 2001-5114	20000313
JP 2002539207	T	20021119	JP 2000-605582	20000313
AU 761453	B2	20030605	AU 2000-31778	20000313
AT 266023	T	20040515	AT 2000-909498	20000313
NZ 514195	A	20040528	NZ 2000-514195	20000313
PT 1163237	T	20040831	PT 2000-909498	20000313
ES 2219319	T3	20041201	ES 2000-909498	20000313
RU 2260007	C2	20050910	RU 2001-128066	20000313
TW 247745	B	20060121	TW 2000-89104783	20000316
ZA 2001007536	A	20030818	ZA 2001-7536	20010912
NO 2001004492	A	20011112	NO 2001-4492	20010914
NO 323191	B1	20070115		
US 7008945	B1	20060307	US 2001-936758	20011115
HK 1041885	A1	20050128	HK 2002-103785	20020521
IN 2004DE02010	A	20070406	IN 2004-DE2010	20041015
IN 2004DN03651	A	20070302	IN 2004-DN3651	20041119
US 2005245551	A1	20051103	US 2005-176327	20050708
US 2006281734	A1	20061214	US 2006-505904	20060818
PRIORITY APPLN. INFO.:				
				GB 1999-6279 A 19990317
				GB 1999-26667 A 19991111
				WO 2000-GB912 W 20000313
				IN 2001-DN827 A3 20010917
				US 2001-936758 A3 20011115
				US 2005-176327 A1 20050708

OTHER SOURCE(S): MARPAT 133:252450
 GI



I



II

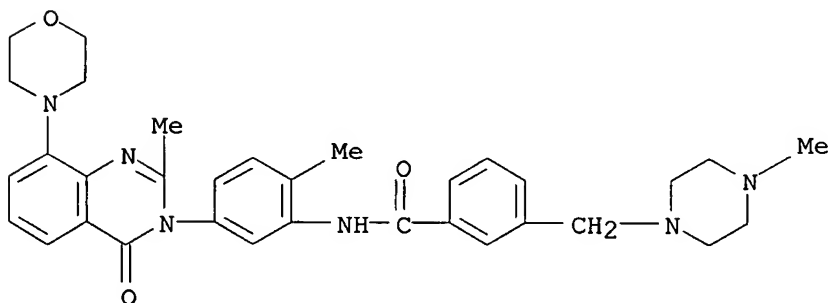
AB The title compds. [I; X = NHCO, CONH; m = 0-3; R1 = OH, halo, CF3, etc.; n = 0-2; R2 = OH, halo, CF3, etc.; R3 = H, halo, alkyl, alkoxy; q = 0-4; Q = aryl, aryloxy, arylalkoxy, etc.], useful in the treatment of diseases or medical conditions mediated by cytokines, were prepared and formulated. E.g., a multi-step synthesis of the quinazolinone II was given. In general compds. I showed over 30% inhibition of p38 α and/or p38 β at up to 10 μ M.

IT 295310-73-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(3-amidophenyl)-3,4-dihydroquinazolin-4-ones for treating diseases mediated by cytokines)

RN 295310-73-5 ZCAPLUS

CN Benzamide, N-[2-methyl-5-[2-methyl-8-(4-morpholinyl)-4-oxo-3(4H)-quinazolinyl]phenyl]-3-[(4-methyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 50 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:311055 ZCAPLUS

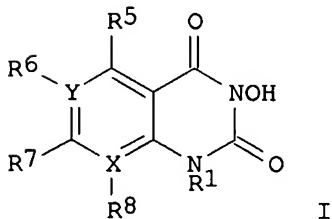
DOCUMENT NUMBER: 130:338119

TITLE: Preparation of 7-substituted 3-hydroxyquinazoline-2,4-

INVENTOR(S): diones and related compounds as antibacterial agents.
Domagala, John Michael; Ellsworth, Edmund Lee; Huang,
Liren; Renau, Thomas Eric; Singh, Rajeshwar; Stier,
Michael Andrew
PATENT ASSIGNEE(S): Warner Lambert Co., USA
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9921840	A1	19990506	WO 1998-US19877	19980923
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9895039	A	19990517	AU 1998-95039	19980923
EP 1028950	A1	20000823	EP 1998-948473	19980923
EP 1028950	B1	20030502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 239000	T	20030515	AT 1998-948473	19980923
PT 1028950	T	20030930	PT 1998-948473	19980923
ES 2195397	T3	20031201	ES 1998-948473	19980923
ZA 9809783	A	19990428	ZA 1998-9783	19981027
US 6331538	B1	20011218	US 2000-508796	20000315
US 2002115674	A1	20020822	US 2001-971343	20011004
US 6825199	B2	20041130		
PRIORITY APPLN. INFO.:			US 1997-63556P	P 19971028
			US 1998-98588P	P 19980831
			WO 1998-US19877	W 19980923
			US 2000-508796	A3 20000315

OTHER SOURCE(S): MARPAT 130:338119
GI

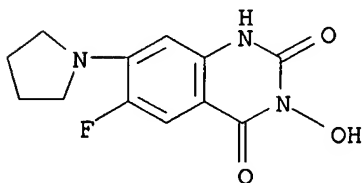


AB Title compds. [I; R1 = H, (substituted) alkyl, cycloalkyl, heterocyclyl, Ph; R5, R6, R8 = H, F, Cl, Br, NO2, cyano, CF3, alkyl, cycloalkyl, amino, etc.; R7 = R5, (substituted) carbocyclyl, Ph, (fused) heterocyclyl, etc.; R1R8 = (substituted) 6-7 membered (heterocyclic) ring; X, Y = C, N]; were prepared Thus, 1-cyclopropyl-6-fluoro-3-hydroxy-7-(pyrrolidin-1-yl)-1H-quinazoline-2,4-dione (preparation given) inhibited Staphylococcus aureus with min. inhibitory concentration = 1.0 µg/mL.
IT 224189-36-0P 224189-37-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 7-substituted 3-hydroxyquinazoline-2,4-diones and related compds. as antibacterial agents)

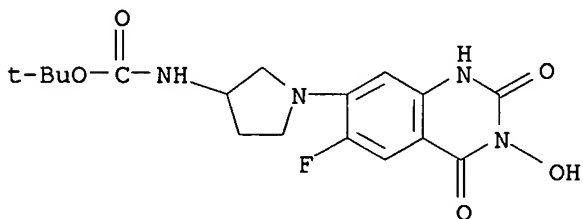
RN 224189-36-0 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-fluoro-3-hydroxy-7-(1-pyrrolidinyl)- (9CI)
(CA INDEX NAME)



RN 224189-37-1 ZCAPLUS

CN Carbamic acid, [1-(6-fluoro-1,2,3,4-tetrahydro-3-hydroxy-2,4-dioxo-7-quinazolinyl)-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



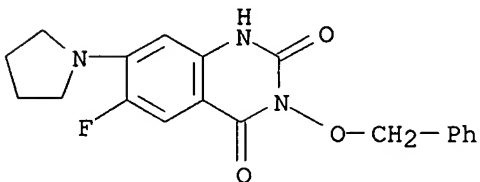
IT 224190-16-3P 224190-17-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 7-substituted 3-hydroxyquinazoline-2,4-diones and related compds. as antibacterial agents)

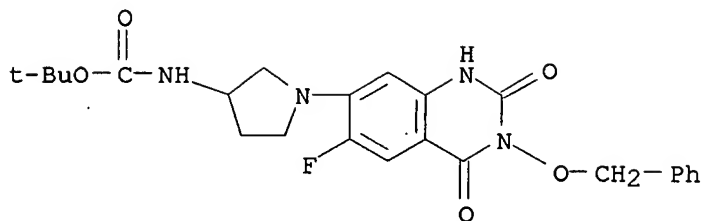
RN 224190-16-3 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-fluoro-3-(phenylmethoxy)-7-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 224190-17-4 ZCAPLUS

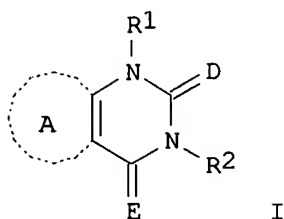
CN Carbamic acid, [1-[6-fluoro-1,2,3,4-tetrahydro-2,4-dioxo-3-(phenylmethoxy)-7-quinazolinyl]-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 51 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:216905 ZCAPLUS
 DOCUMENT NUMBER: 130:252369
 TITLE: Preparation and formulation of quinazoline derivatives as allergy inhibitors
 INVENTOR(S): Kajino, Masahiro; Morimoto, Shinji; Inaba, Atsuhiko; Nagaya, Hideaki
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
 SOURCE: PCT Int. Appl., 324 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9914203	A1	19990325	WO 1998-JP4103	19980911
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2302453	A1	19990325	CA 1998-2302453	19980911
AU 9890025	A	19990405	AU 1998-90025	19980911
JP 11152275	A	19990608	JP 1998-257761	19980911
EP 1026160	A1	20000809	EP 1998-941835	19980911
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6407116	B1	20020618	US 2000-486646	20000225
PRIORITY APPLN. INFO.:			JP 1997-250960	A 19970916
			WO 1998-JP4103	W 19980911
OTHER SOURCE(S):			MARPAT 130:252369	
GI				



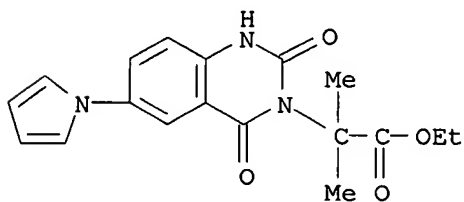
AB The title compds. I [A is a (substituted) homocycle or nitrogenous heterocycle; D and E are each O or S; and one of R1 and R2 is a group represented by general formula XBYC(R3)(Ar1)(Ar2); Ar1 and Ar2 are each a (substituted) aromatic group or they together with the carbon atom adjacent to them may form a (substituted) fused-ring group; B is a (substituted) nitrogenous heterocycle; X and Y are each a bond, O, S(O)p (wherein p is an integer of 0 to 2), NR4 (wherein R4 is H or lower alkyl) or a divalent (substituted) linear lower hydrocarbon group optionally interrupted by a heteroatom; and R3 is H, (substituted) hydroxyl or (esterified) carboxyl, and the other of them is H, cyano or a (substituted) hydrocarbon group] are prepared I are antihistaminics and eosinophilic chemotaxis inhibitors and are useful in the treatment of asthma, allergic conjunctivitis, allergic rhinitis, urticaria, atopic dermatitis, etc.
2,4-Dioxo-1-[4-(4-diphenylmethoxy-1-piperidinyl)butyl]-1,2,3,4-tetrahydroquinazoline in vitro at 1×10^{-5} M gave 91% inhibition of LTB4-induced chemotaxis.

IT 221541-27-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinazoline derivs. as allergy inhibitors)

RN 221541-27-1 ZCAPLUS

CN 3(2H)-Quinazolineacetic acid, 1,4-dihydro- α,α -dimethyl-2,4-dioxo-6-(1H-pyrrol-1-yl)-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 52 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:48710 ZCAPLUS

DOCUMENT NUMBER: 130:125085

TITLE: Preparation of quinazoline analogs and related compounds for treating inflammatory conditions

INVENTOR(S): Palanki, Moorthy S. S.; Suto, Mark J.

PATENT ASSIGNEE(S): Signal Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

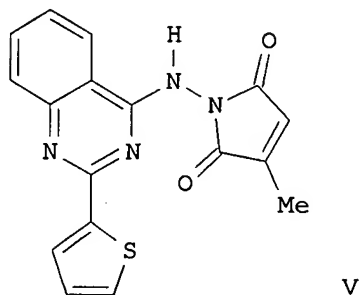
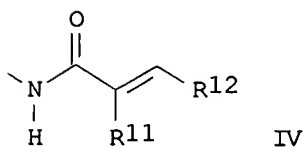
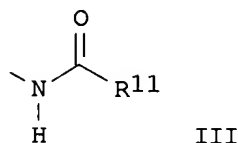
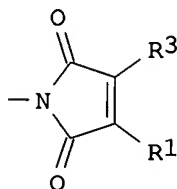
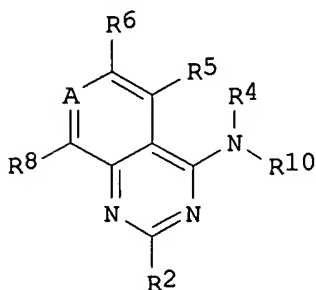
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9901441	A1	19990114	WO 1998-US13483	19980629
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5939421	A	19990817	US 1997-886198	19970701
AU 9881754	A	19990125	AU 1998-81754	19980629
US 6150372	A	20001121	US 1999-340557	19990628
PRIORITY APPLN. INFO.:			US 1997-886198	A 19970701
			WO 1998-US13483	W 19980629
OTHER SOURCE(S):	MARPAT 130:125085			
GI				



AB The title compds. [I; R10 = II-IV; A = CR7, N; R1, R3 = H, (un)substituted C1-8 alkyl, C6-12 aryl; R2 = (un)substituted C1-8 alkyl, C6-12 aryl, etc.; R4 = H, C1-8 alkyl; R5-R8 = H, NO2, CN, etc.; R11 = H, (un)substituted C1-8 alkyl, C6-12 aryl; R12 = H, CO2R9, CONHR9; R9 = H, (un)substituted C1-8 alkyl, C6-12 aryl, etc.], having utility as anti-inflammatory agents in general and, more specifically, for the prevention and/or treatment of immunoinflammatory (such as rheumatoid arthritis, rheumatoid arthritis, rheumatoid arthritis, osteoarthritis, transplant rejection, sepsis, ARDS, and asthma) and autoimmune diseases (such as multiple sclerosis, psoriasis, inflammatory bowel disease, glomerulonephritis, uveitis, and chronic hepatitis), and trauma, oxidative stress, cell death, irradiation damage, ischemia, reperfusion, cancer and viral infection, were prepared Thus, reaction of 4-chloro-2-(2'-thienyl)quinazoline (preparation given) with hydrazine in THF followed by treatment of the resulting intermediate with

citraconic anhydride in chloroform afforded 98% V which showed IC₅₀ of 0.07 μ M against AP-1 and IC₅₀ of 0.04 μ M against NF κ B.

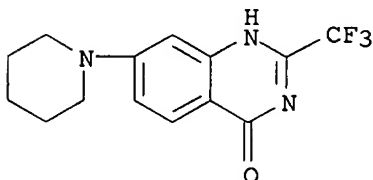
IT 219774-02-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinazoline analogs and related compds. for treating inflammatory conditions)

RN 219774-02-4 ZCAPLUS

CN 4(1H)-Quinazolinone, 7-(1-piperidinyl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 53 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:490639 ZCAPLUS

DOCUMENT NUMBER: 129:136176

TITLE: Quinoline and quinazoline compounds useful in therapy, particularly in the treatment of benign prostatic hyperplasia

INVENTOR(S): Fox, David Nathan Abraham

PATENT ASSIGNEE(S): Pfizer Ltd., UK; Pfizer Inc.; Fox, David Nathan Abraham

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

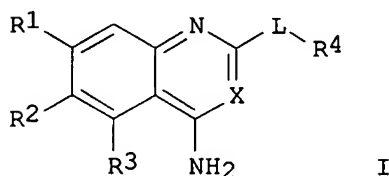
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9830560	A1	19980716	WO 1998-EP143	19980106
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
TW 444013	B	20010701	TW 1997-86117203	19971118
CA 2277473	A1	19980716	CA 1998-2277473	19980106
CA 2277473	C	20030812		
EP 968208	A1	20000105	EP 1998-904058	19980106
EP 968208	B1	20030604		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AP 819	A	20000403	AP 1998-1175	19980106
W: BW, GM, KE, MW, UG, ZM, ZW				
JP 2000507966	T	20000627	JP 1998-530565	19980106
JP 3357677	B2	20021216		

NZ 336302	A	20000825	NZ 1998-336302	19980106
HU 200000942	A2	20010428	HU 2000-942	19980106
CN 1093858	B	20021106	CN 1998-801748	19980106
AT 242238	T	20030615	AT 1998-904058	19980106
PT 968208	T	20030930	PT 1998-904058	19980106
ES 2198695	T3	20040201	ES 1998-904058	19980106
CZ 295580	B6	20050817	CZ 1999-2436	19980106
SK 284779	B6	20051103	SK 1999-907	19980106
IL 130762	A	20051218	IL 1998-130762	19980106
HR 980010	B1	20020630	HR 1998-10	19980108
BG 63918	B1	20030630	BG 1999-103560	19990707
NO 9903396	A	19990709	NO 1999-3396	19990709
NO 318609	B1	20050418		
US 6365599	B1	20020402	US 2000-586503	20000602
HK 1025327	A1	20030711	HK 2000-104585	20000724
US 2002040028	A1	20020404	US 2001-7753	20011113
US 6521629	B2	20030218		
CN 1403453	A	20030319	CN 2001-143291	20011226
US 2003130259	A1	20030710	US 2002-318902	20021213
US 6653302	B2	20031125		
HK 1054389	A1	20051014	HK 2003-106677	20030917
PRIORITY APPLN. INFO.:			GB 1997-504	A 19970111
			WO 1998-EP143	W 19980106
			US 1999-341228	A3 19990707
			US 2000-586503	A3 20000602
			US 2001-7753	A3 20011113

OTHER SOURCE(S): MARPAT 129:136176
GI

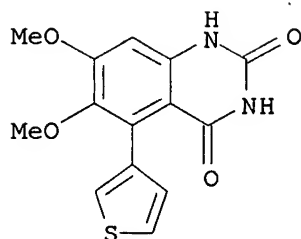


AB I [R1 = C1-4 alkoxy optionally substituted by one or more fluorine atoms; R2 = H, C1-6 alkoxy optionally substituted by one or more fluorine atoms; R3 = 5- or 6-membered heterocyclic ring, the ring being optionally substituted; R4 = 4-, 5-, 6- or 7-membered heterocyclic ring, the ring being optionally fused to a benzene ring or a 5- or 6-membered heterocyclic ring, the ring system as a whole being optionally substituted; X = CH, N; L is absent or represents a N-containing cyclic group or chain], useful in treatment of benign prostatic hyperplasia, were prepared E.g., 4-amino-6,7-dimethoxy-2-[4-(4-morpholinecarbonyl)-1,4-diazepan-1-yl]-5-(oxazol-2-yl)quinoline was prepared

IT 210538-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinoline and quinazoline derivs. useful in treatment of benign prostatic hyperplasia)

RN 210538-64-0 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6,7-dimethoxy-5-(3-thienyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 54 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:772565 ZCAPLUS

DOCUMENT NUMBER: 123:169645

TITLE: Angiotensin II receptor blocking [(biphenyl)yl)methyl]quinazolinones.

INVENTOR(S): Levin, Jeremy I.; Venkatesan, Aranapakam M.

PATENT ASSIGNEE(S): American Cyanamid Co., USA

SOURCE: Eur. Pat. Appl., 132 pp.

CODEN: EPXXDW

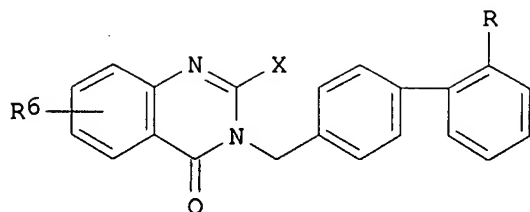
DOCUMENT TYPE: Patent

LANGUAGE: English

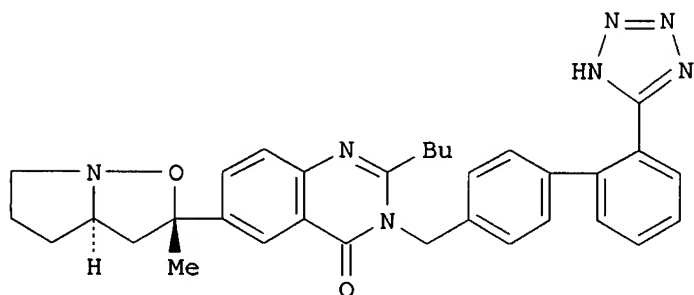
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 621276	A1	19941026	EP 1994-105285	19940405
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 5358951	A	19941025	US 1993-52945	19930423
CA 2121897	A1	19941024	CA 1994-2121897	19940421
JP 07025870	A	19950127	JP 1994-106216	19940422
PRIORITY APPLN. INFO.:			US 1993-52945	A 19930423
OTHER SOURCE(S):	MARPAT 123:169645			
GI				



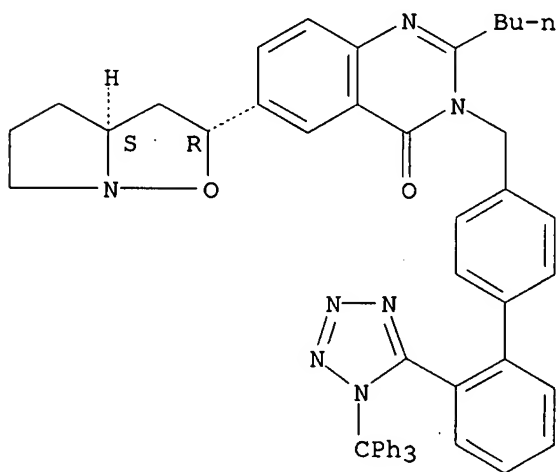
I



II

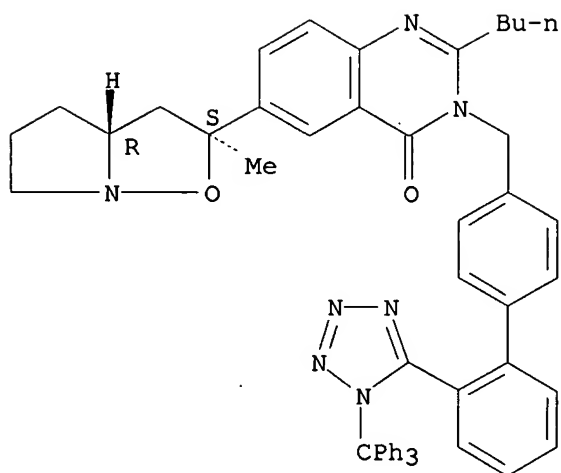
- AB The 3-(biphenylmethyl)-4-quinazolinones I (R = tetrazolyl, carboxy, sulfonylamino; R₆ = (un)substituted Ph, etc.) were disclosed as angiotensin II (AII) antagonists. The example compound II was prepared
- IT 155995-19-0P 155995-49-6P 155995-56-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of (biphenylmethyl)quinazolinones angiotensin antagonists)
- RN 155995-19-0 ZCAPLUS
- CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



- RN 155995-49-6 ZCAPLUS
- CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

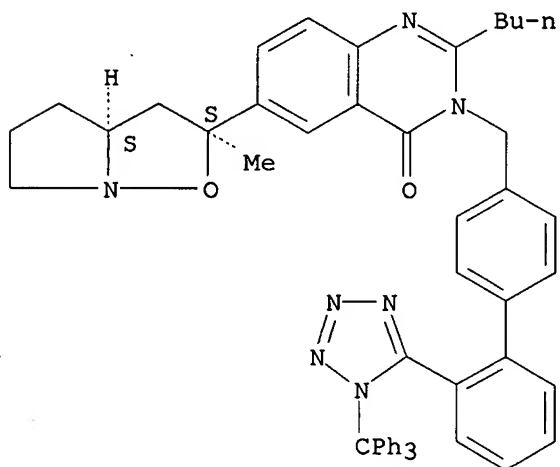
Relative stereochemistry.



RN 155995-56-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



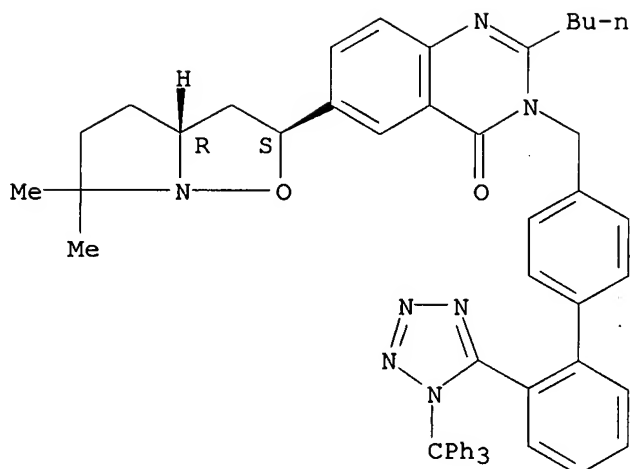
IT 155995-22-5P 155995-23-6P 155995-27-0P
 155995-28-1P 155995-29-2P 155995-30-5P
 155995-31-6P 155995-32-7P 155995-34-9P
 155995-35-0P 155995-36-1P 155995-40-7P
 155995-41-8P 155995-42-9P 155995-43-0P
 155995-45-2P 155995-47-4P 155995-49-6P
 155995-53-2P 159969-27-4P 159969-28-5P
 159969-30-9P 167301-39-5P 167301-40-8P
 167301-41-9P 167301-42-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of (biphenylmethyl)quinazolinones angiotensin antagonists)

RN 155995-22-5 ZCAPLUS

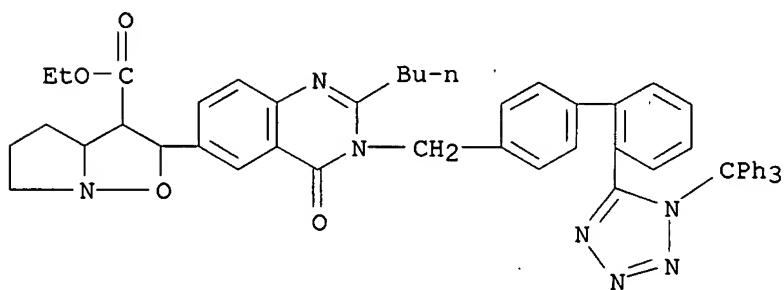
CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155995-23-6 ZCAPLUS

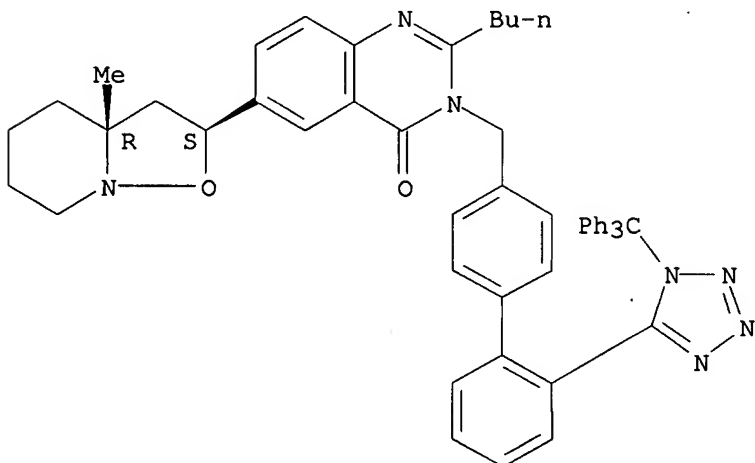
CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, ethyl ester (9CI) (CA INDEX NAME)



RN 155995-27-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-3a-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

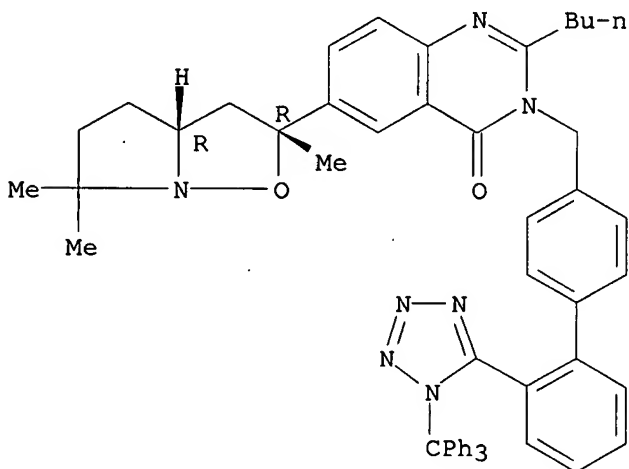
Relative stereochemistry.



RN 155995-28-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

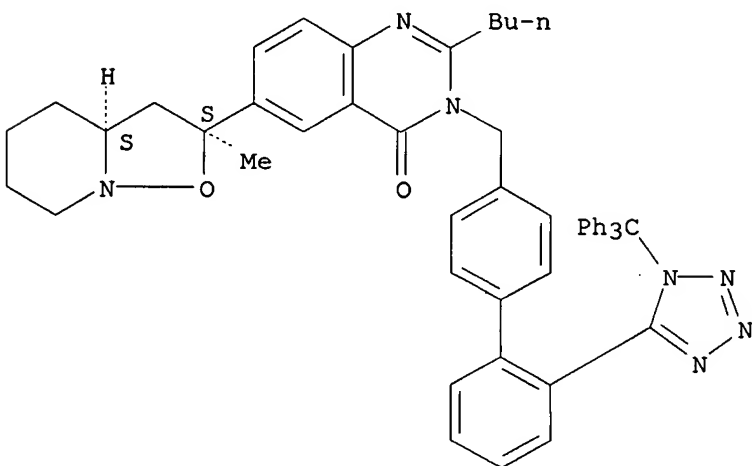
Relative stereochemistry.



RN 155995-29-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

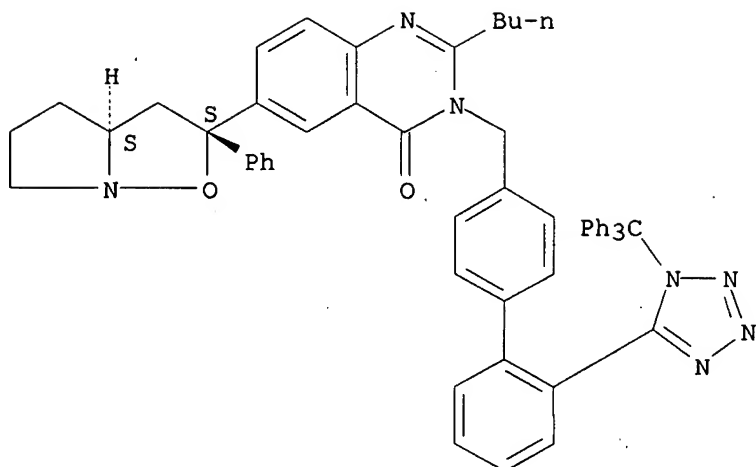
Relative stereochemistry.



RN 155995-30-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-phenylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

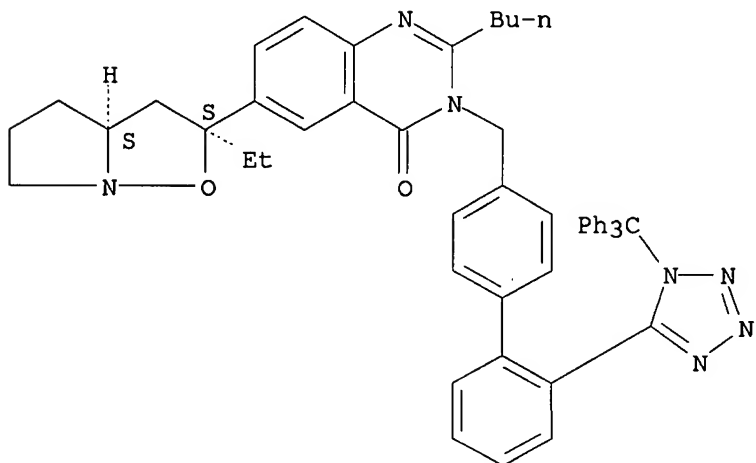
Relative stereochemistry.



RN 155995-31-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

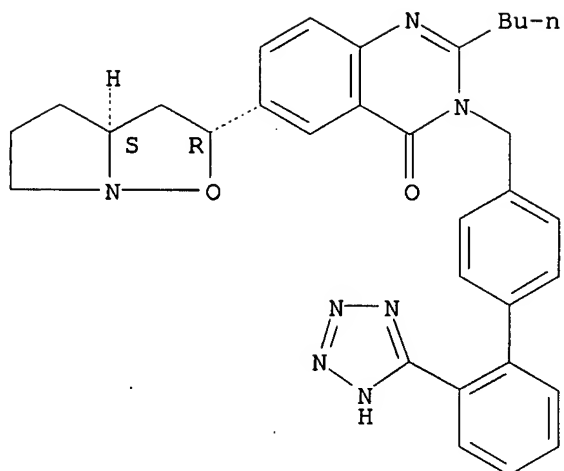
Relative stereochemistry.



RN 155995-32-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

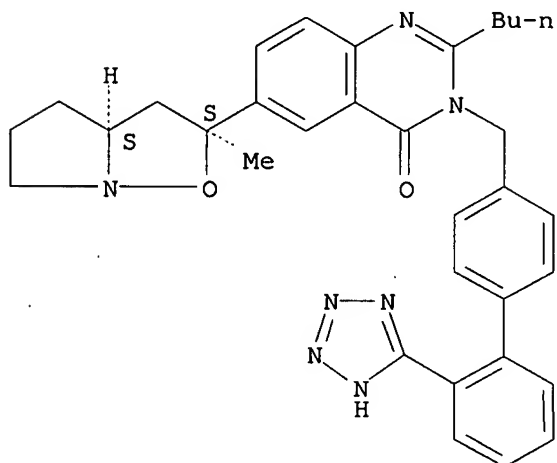
Relative stereochemistry.



RN 155995-34-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

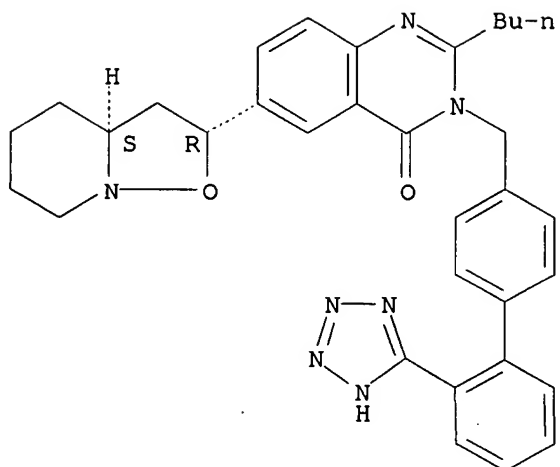
Relative stereochemistry.



RN 155995-35-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

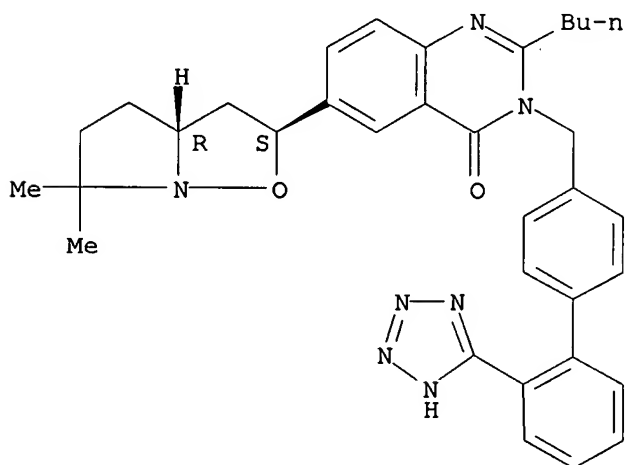
Relative stereochemistry.



RN 155995-36-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

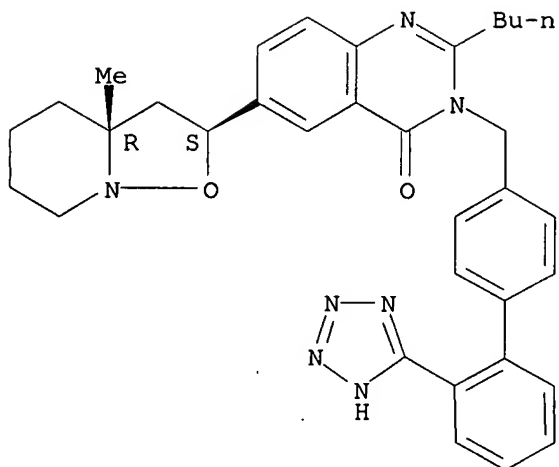
Relative stereochemistry.



RN 155995-40-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-3a-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

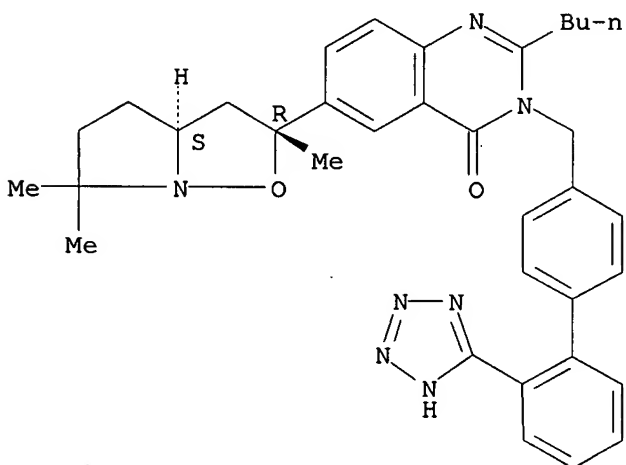
Relative stereochemistry.



RN 155995-41-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

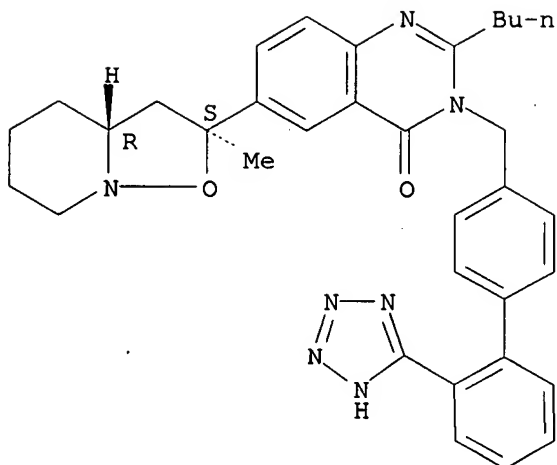
Relative stereochemistry.



RN 155995-42-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

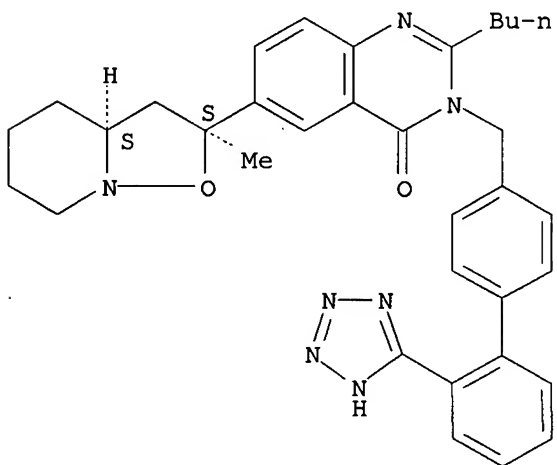
Relative stereochemistry.



RN 155995-43-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

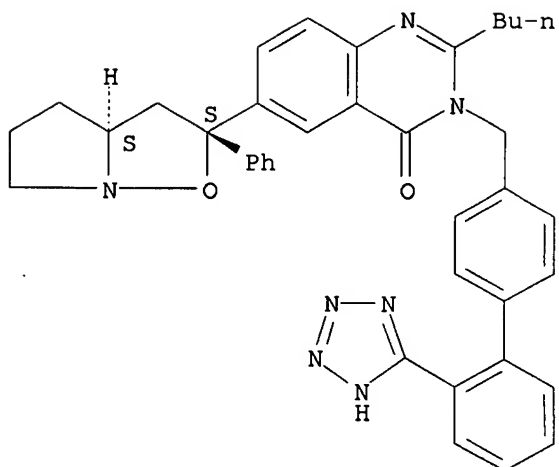
Relative stereochemistry.



RN 155995-45-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-phenylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

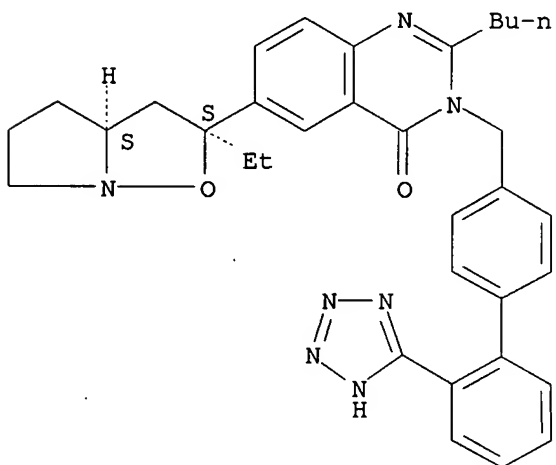
Relative stereochemistry.



RN 155995-47-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

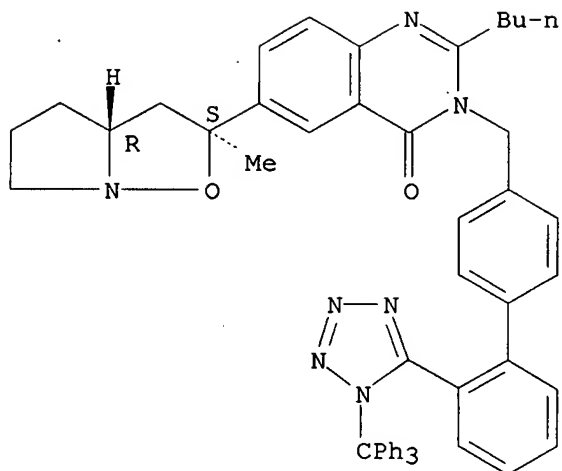
Relative stereochemistry.



RN 155995-49-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

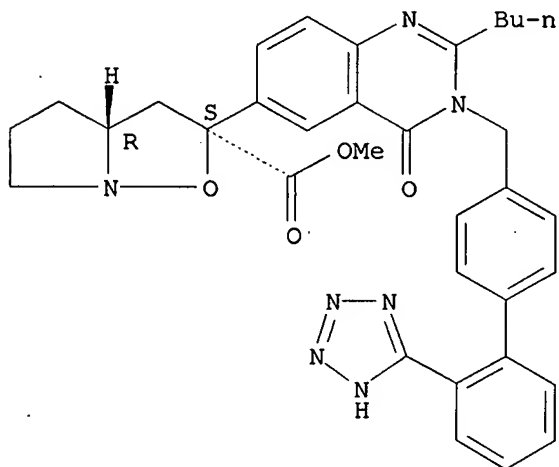
Relative stereochemistry.



RN 155995-53-2 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

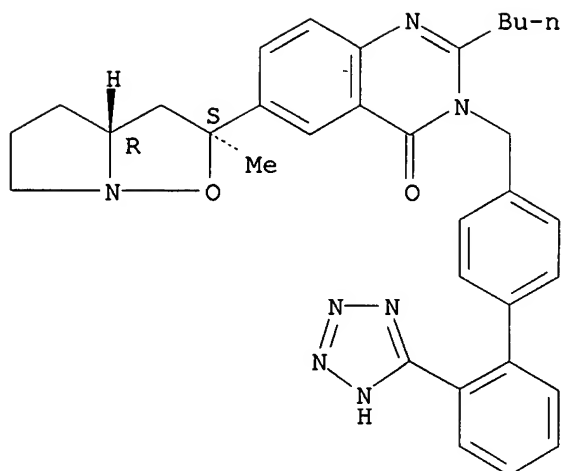
Relative stereochemistry.



RN 159969-27-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

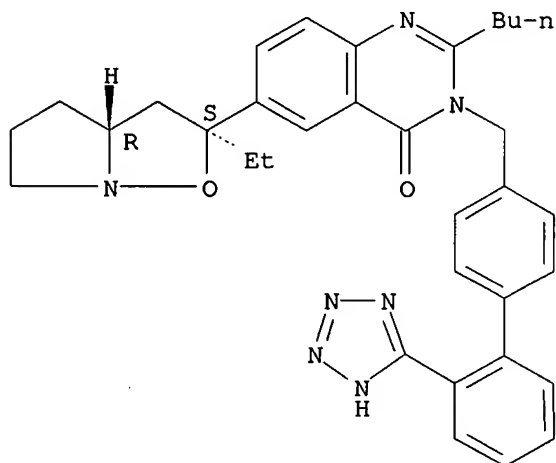
Relative stereochemistry.



RN 159969-28-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI)
(CA INDEX NAME)

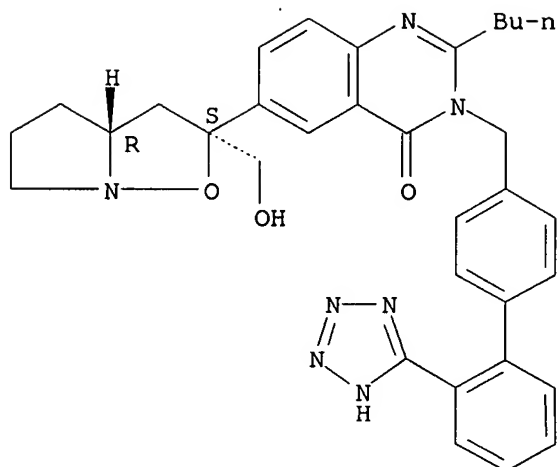
Relative stereochemistry.



RN 159969-30-9 ZCAPLUS

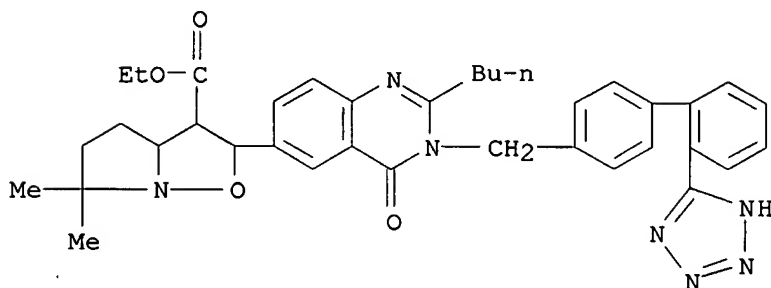
CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 167301-39-5 ZCAPLUS

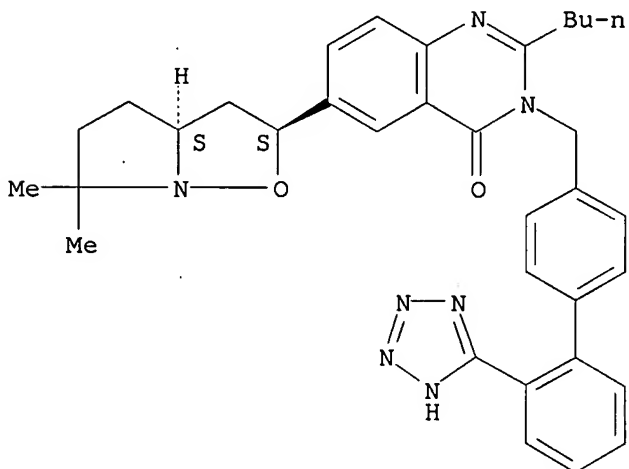
CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-6,6-dimethyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 167301-40-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

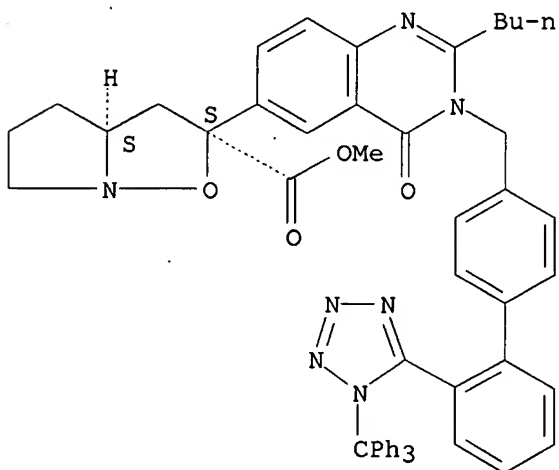
Relative stereochemistry.



RN 167301-41-9 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, cis- (9CI) (CA INDEX NAME)

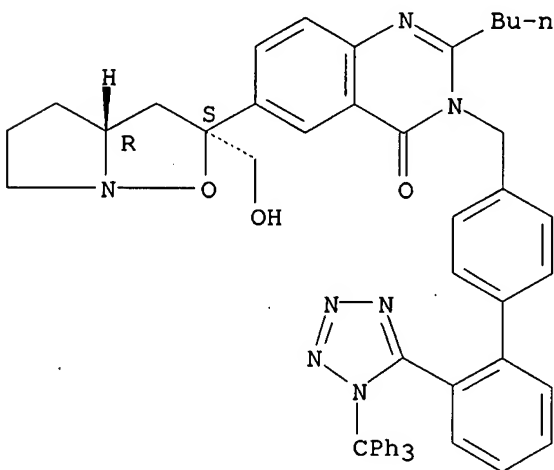
Relative stereochemistry.



RN 167301-42-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[(2R,3aS)-hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



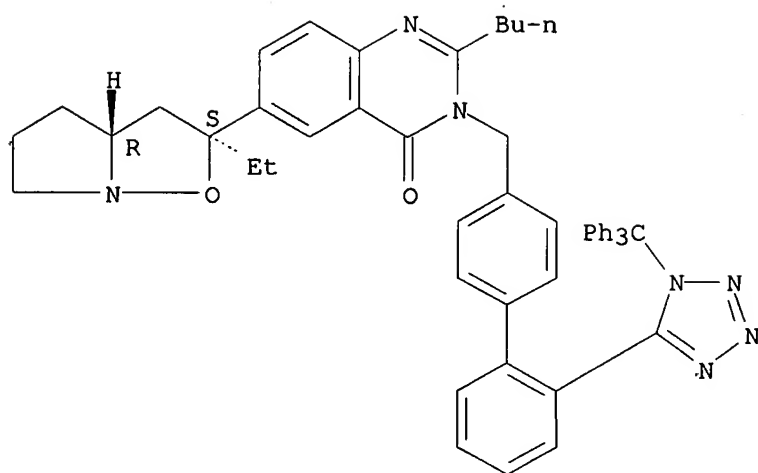
IT 155995-46-3 155995-55-4 167301-38-4

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of (biphenylmethyl)quinazolinones angiotensin antagonists)

RN 155995-46-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

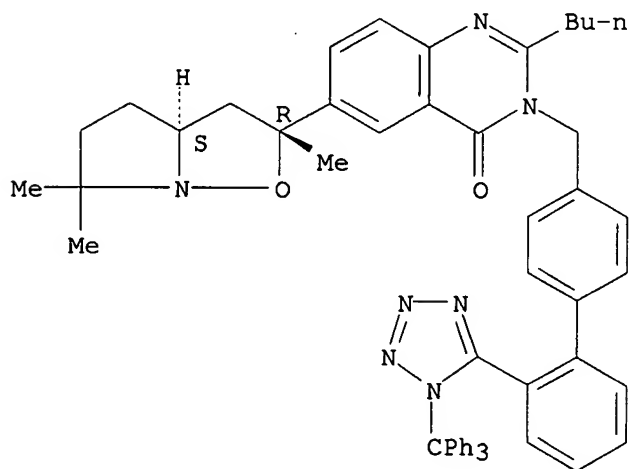
Relative stereochemistry.



RN 155995-55-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

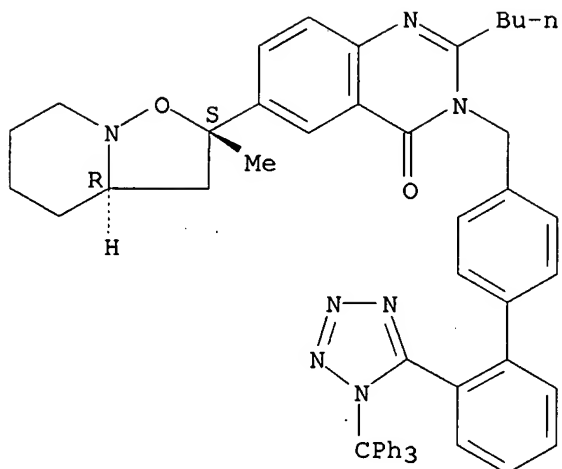
Relative stereochemistry.



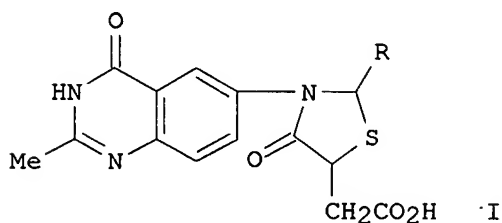
RN 167301-38-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 55 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:419771 ZCAPLUS
 DOCUMENT NUMBER: 123:55750
 TITLE: 4-Thiazolidinones: Part XXI. 6-(2'-Aryl-5'-carboxymethyl-4'-thiazolidinon-3'-yl)-2-methyl-4(3H)-quinazolinone
 AUTHOR(S): Vyas, Arti; Joshi, H. S.; Parekh, Hansa
 CORPORATE SOURCE: Chemistry Department, Saurashtra University, Rajkot, 360 005, India
 SOURCE: Journal of the Institution of Chemists (India) (1994), 66(2), 41-2
 CODEN: JOICA7; ISSN: 0020-3254
 PUBLISHER: Institution of Chemists (India)
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123:55750
 GI



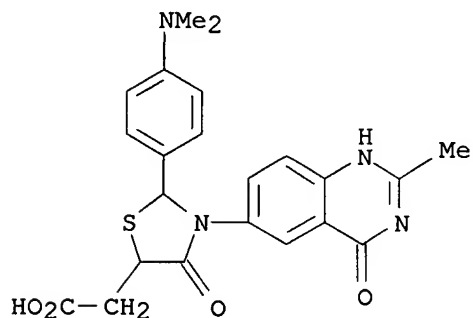
AB The title compds. I [R = (un)substituted Ph, 2-furyl, cinnamyl] were prepared by reaction of 6-amino-2-methyl-4(3H)-quinazolinone with aromatic aldehydes, followed by reaction with thiomalic acid. I showed moderate bactericidal and fungicidal activities.
 IT 164587-12-6P 164587-13-7P 164587-14-8P
 164587-15-9P 164587-16-0P 164587-17-1P
 164587-18-2P 164587-19-3P 164587-20-6P
 164587-21-7P 164587-22-8P 164587-23-9P
 164587-24-0P 164587-25-1P 164587-26-2P
 164587-27-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and bactericidal and fungicidal activities of thiazolidinonylquinazolinones)

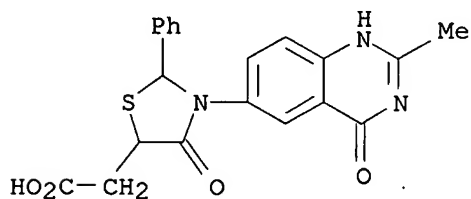
RN 164587-12-6 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-[4-(dimethylamino)phenyl]-4-oxo- (9CI) (CA INDEX NAME)



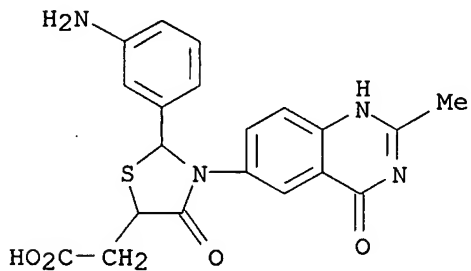
RN 164587-13-7 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo-2-phenyl- (9CI) (CA INDEX NAME)



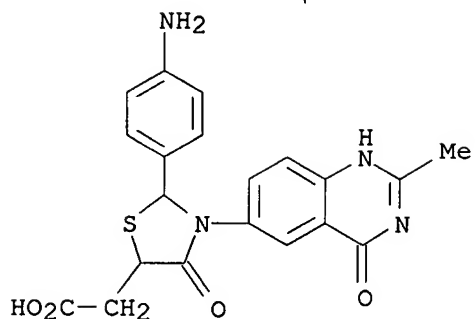
RN 164587-14-8 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(3-aminophenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



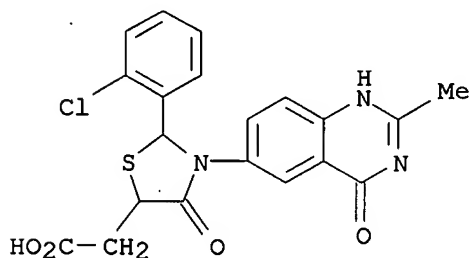
RN 164587-15-9 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(4-aminophenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



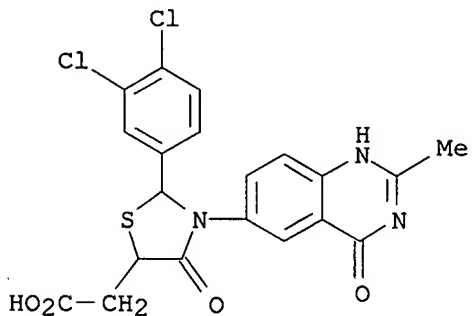
RN 164587-16-0 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(2-chlorophenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



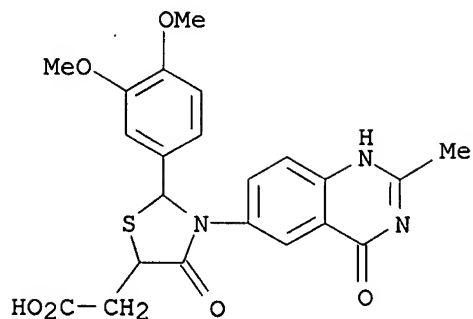
RN 164587-17-1 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(3,4-dichlorophenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



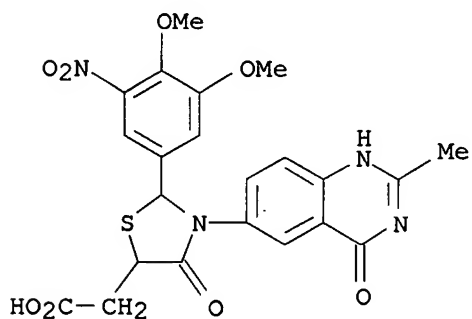
RN 164587-18-2 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(3,4-dimethoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



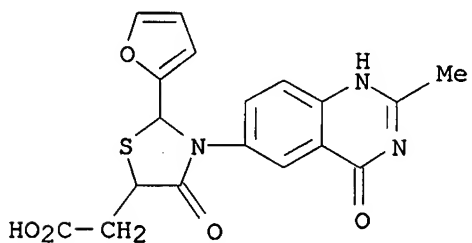
RN 164587-19-3 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(3,4-dimethoxy-5-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)



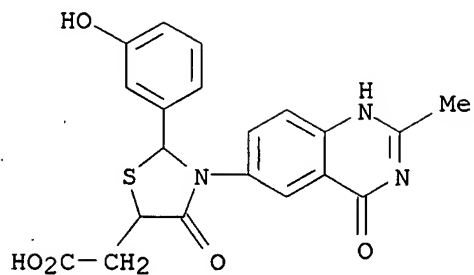
RN 164587-20-6 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(2-furanyl)-4-oxo- (9CI) (CA INDEX NAME)



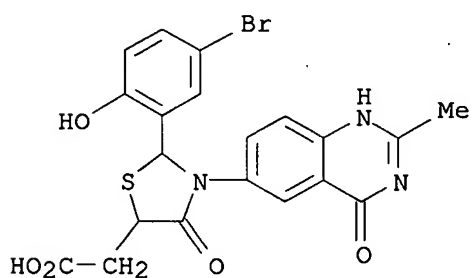
RN 164587-21-7 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(3-hydroxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



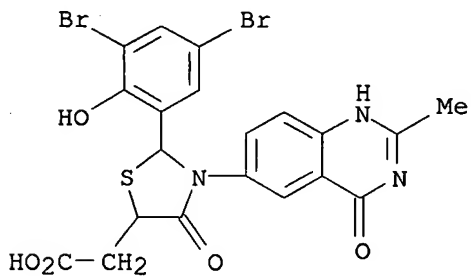
RN 164587-22-8 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(5-bromo-2-hydroxyphenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



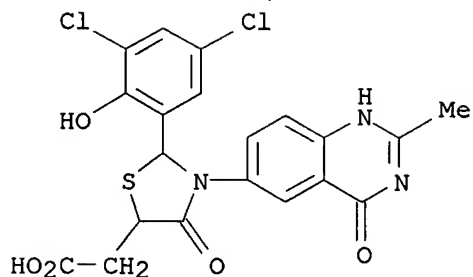
RN 164587-23-9 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(3,5-dibromo-2-hydroxyphenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



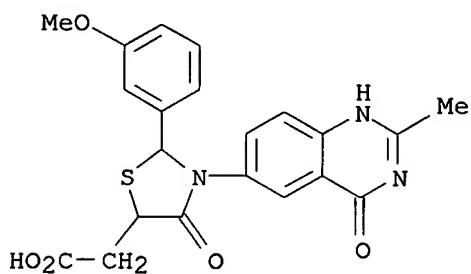
RN 164587-24-0 ZCAPLUS

CN 5-Thiazolidineacetic acid, 2-(3,5-dichloro-2-hydroxyphenyl)-3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo- (9CI) (CA INDEX NAME)



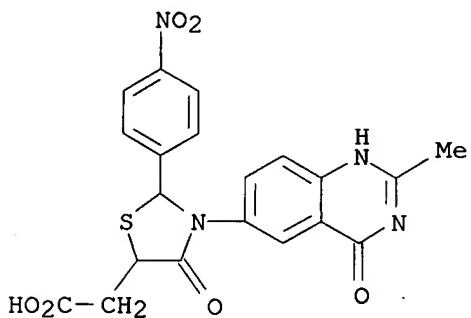
RN 164587-25-1 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(3-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



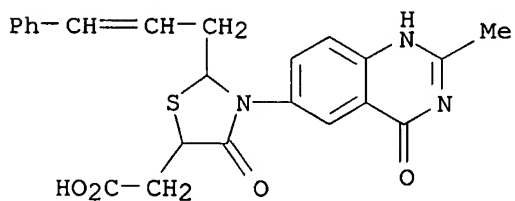
RN 164587-26-2 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-2-(4-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)



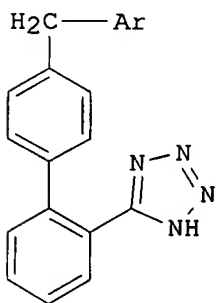
RN 164587-27-3 ZCAPLUS

CN 5-Thiazolidineacetic acid, 3-(1,4-dihydro-2-methyl-4-oxo-6-quinazolinyl)-4-oxo-2-(3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 56 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:397363 ZCAPLUS
 DOCUMENT NUMBER: 123:276050
 TITLE: Angiotensin II (AII) antagonists as inhibitors of the growth of adipose tissue
 INVENTOR(S): Crandall, David Leroy
 PATENT ASSIGNEE(S): American Cyanamid Co., USA
 SOURCE: Eur. Pat. Appl., 40 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 635263	A2	19950125	EP 1994-108298	19940530
EP 635263	A3	19950927		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07017862	A	19950120	JP 1994-164687	19940623
CA 2126709	A1	19941229	CA 1994-2126709	19940624
AU 9465991	A	19950105	AU 1994-65991	19940627
AU 680659	B2	19970807		
US 5830909	A	19981103	US 1996-684609	19960719
PRIORITY APPLN. INFO.:			US 1993-82562	A 19930628
OTHER SOURCE(S):	MARPAT 123:276050			
GI				



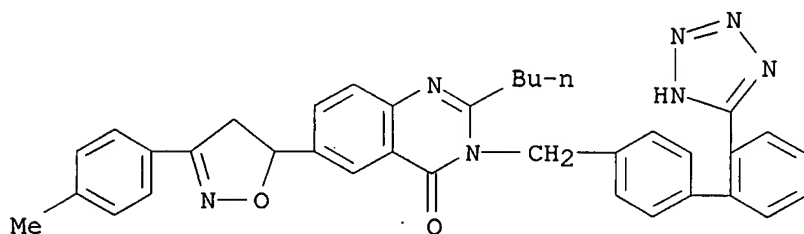
I

AB AII receptor-blocking tetrazolylbiphenyl compds. I (Ar = N-containing heterocycle) and related compds. are useful for inhibiting adipocyte AII receptors and thereby reducing adipocyte growth and body weight gain and for treatment of associated diseases, e.g. obesity and noninsulin-dependent diabetes mellitus. Binding characteristics of the adipocyte membrane AII receptors in rats and humans were determined. Thus, 2-ethyl-5,7-dimethyl-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-3H-imidazo[4,5-b]pyridine displaced 125I-labeled [Sar1,Ile8]angiotensin II from rat epididymal fat cell membranes with an IC_{50} of $2.44 \pm 10^{-9}\text{M}$.

IT 154749-04-9 154749-08-3 155995-53-2
 157897-47-7 161443-48-7 161443-49-8
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (angiotensin II antagonists as inhibitors of growth of adipose tissue)

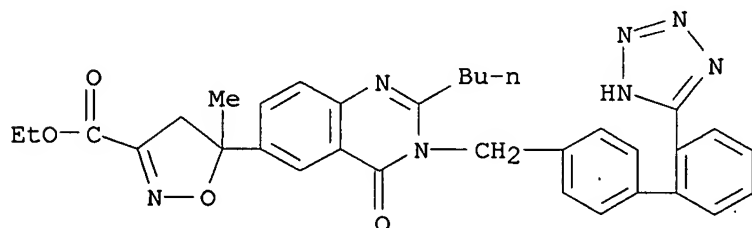
RN 154749-04-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methylphenyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



RN 154749-08-3 ZCAPLUS

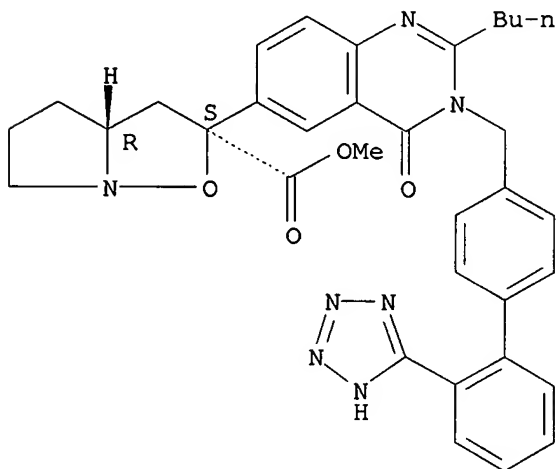
CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 155995-53-2 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

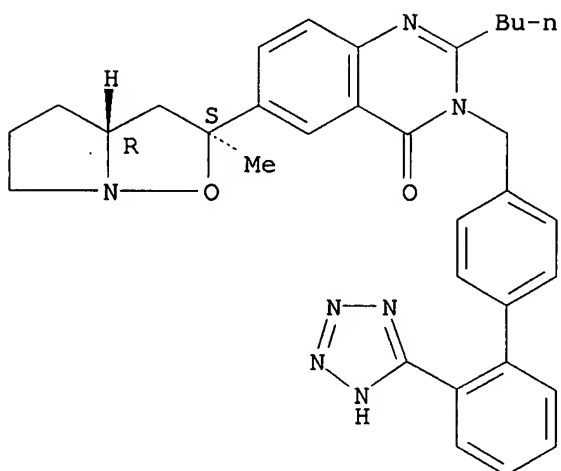
Relative stereochemistry.



RN 157897-47-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

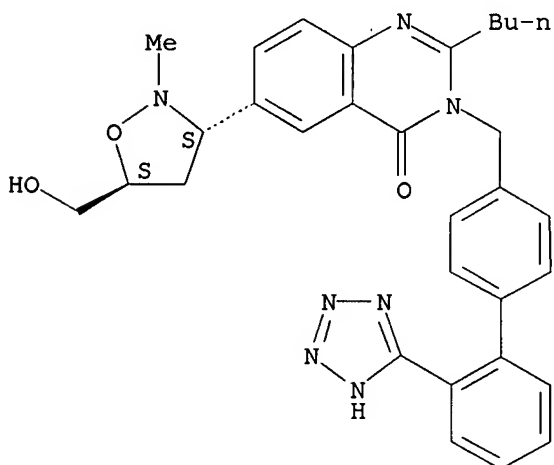


● Na

RN 161443-48-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3S-trans)- (9CI) (CA INDEX NAME)

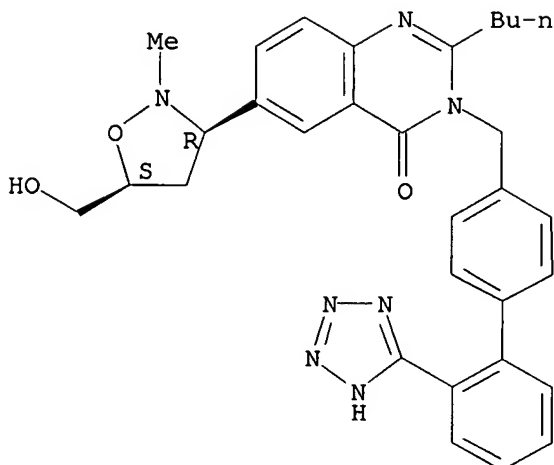
Absolute stereochemistry.



RN 161443-49-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 57 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:230091 ZCAPLUS

DOCUMENT NUMBER: 122:23227

TITLE: Derivation of a 3D pharmacophore model for the angiotensin-II site one receptor

AUTHOR(S): Prendergast, Kristine; Adams, Kym; Greenlee, William J.; Nachbar, Robert B.; Patchett, Arthru A.; Underwood, Dennis J.

CORPORATE SOURCE: Mol. Systems Dep., Merck Res. Lab., Rahway, NJ, 07065, USA

SOURCE: Journal of Computer-Aided Molecular Design (1994), 8(5), 491-512

CODEN: JCADEQ; ISSN: 0920-654X

PUBLISHER: ESCOM

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A systematic search has been use to derive a hypothesis for the receptor-bound conformation of A-II antagonists at the AT1 receptor. The validity of the pharmacophore hypothesis has been tested using CoMFA, which included 50 diverse A-II antagonists, spanning four orders of magnitude in activity. The resulting cross-validated R2 or 0.64 (conventional R2 of 0.76) is indicative of a good predictive model of activity, and has been used to estimate potency for a variety of non-peptidyl antagonists. The structural model for the non-peptide has been compared with respect to the natural substrate, A-II, by generating peptide to non-peptide overlays.

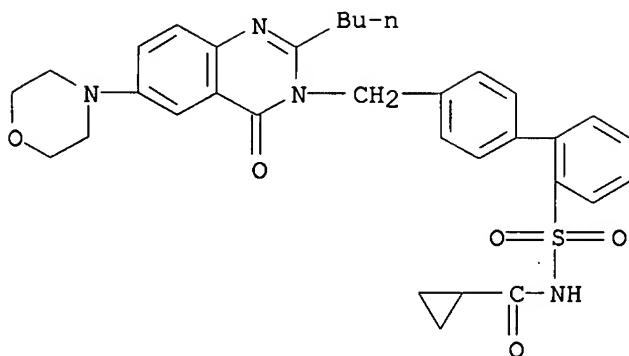
IT 150004-49-2 159859-82-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

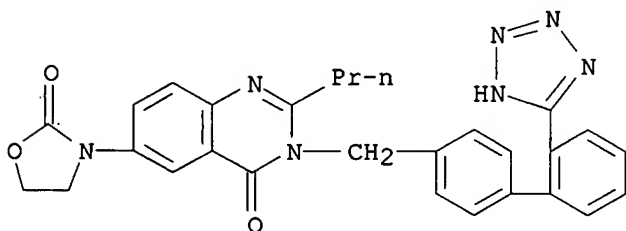
(derivation of a 3D pharmacophore model for the angiotensin-II site one receptor)

RN 150004-49-2 ZCAPLUS

CN Cyclopropanecarboxamide, N-[[4'-[[2-butyl-6-(4-morpholinyl)-4-oxo-3(4H)-quinazolinyl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 159859-82-2 ZCAPLUS
 CN 4(3H)-Quinazolinone, 6-(2-oxo-3-oxazolidinyl)-2-propyl-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 58 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:44916 ZCAPLUS

DOCUMENT NUMBER: 122:55978

TITLE: 6-Substituted quinazolinone angiotensin II receptor antagonists

AUTHOR(S): Levin, J. I.; Venkatesan, A. M.; Chan, P. S.; Bailey, T. K.; Vice, G.; Coupet, J.

CORPORATE SOURCE: Med. Res. Div., American Cyanamid Company, Pearl River, NY, 10965, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(15), 1819-24

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 4(3H)-quinazolinones with a variety of heterocyclic substituents bound to the 6-position have been synthesized and evaluated as angiotensin II receptor antagonists both in vitro and in vivo. Some of these compds. have been shown to be potent, long-lasting, orally active antihypertensives.

IT 155879-19-9P 155879-20-2P 158293-37-9P
 159039-86-8P 159040-08-1P 159040-13-8P
 159040-15-0P 159168-90-8P 159168-91-9P
 160058-73-1P 160058-75-3P 160167-90-8P
 160167-92-0P 160167-93-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

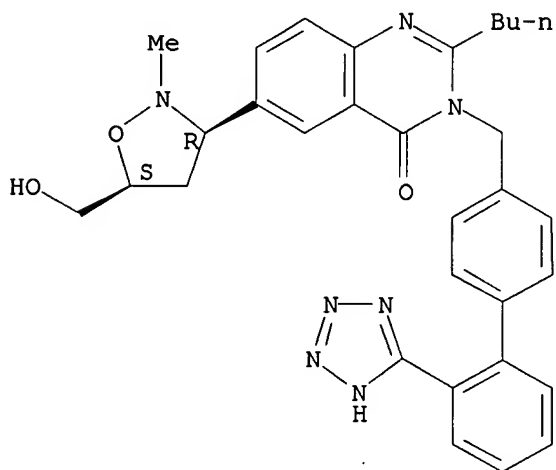
(preparation of heterocyclyl-substituted quinazolinones as angiotensin II receptor antagonists)

RN 155879-19-9 ZCAPLUS

10/ 530,897

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

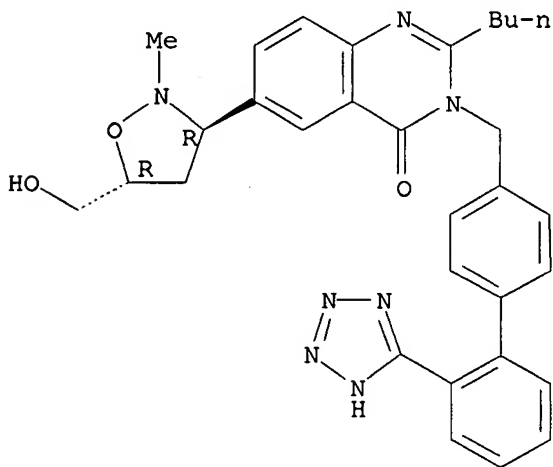
Relative stereochemistry.



RN 155879-20-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

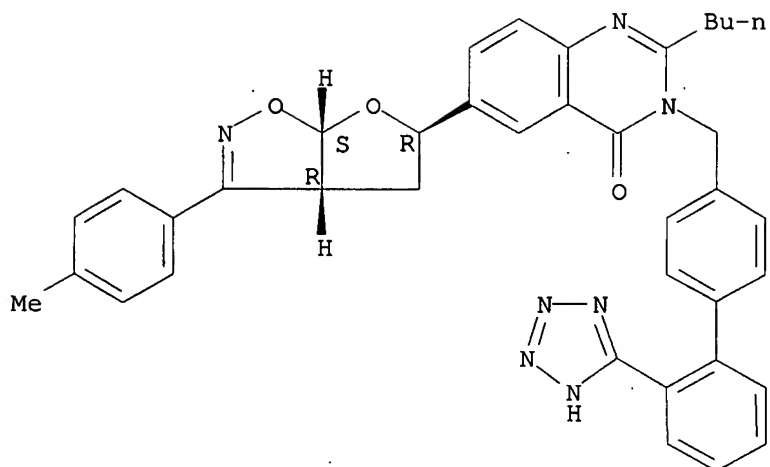
Relative stereochemistry.



RN 158293-37-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[3a,4,5,6a-tetrahydro-3-(4-methylphenyl)furo[3,2-d]isoxazol-5-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3a α ,5 α ,6a α)- (9CI) (CA INDEX NAME)

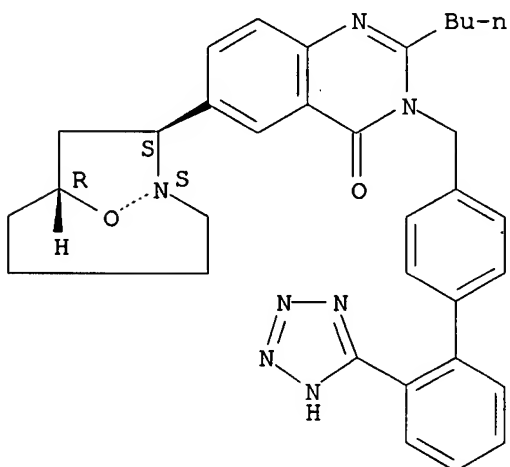
Relative stereochemistry.



RN 159039-86-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(9-oxa-1-azabicyclo[4.2.1]non-8-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, exo- (9CI) (CA INDEX NAME)

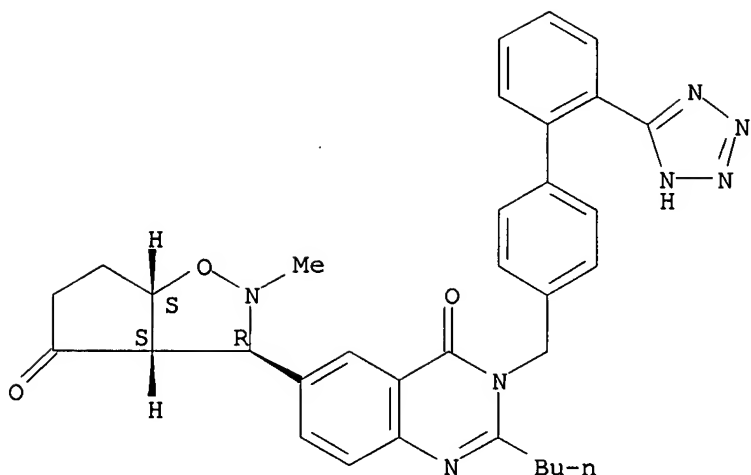
Relative stereochemistry.



RN 159040-08-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxo-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3α,6α)- (9CI) (CA INDEX NAME)

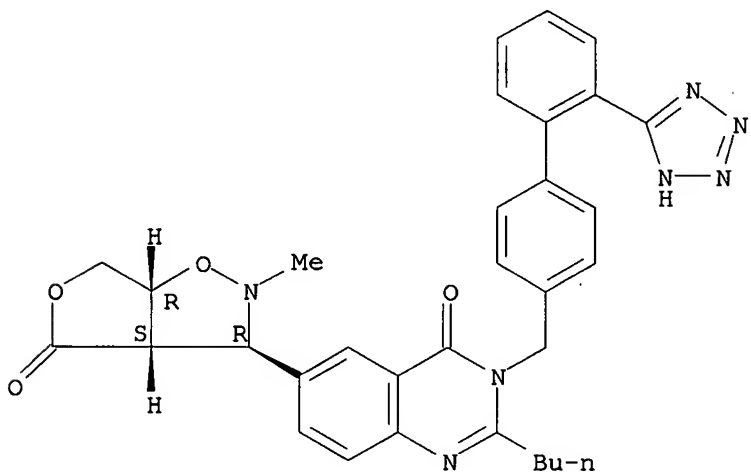
Relative stereochemistry.



RN 159040-13-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

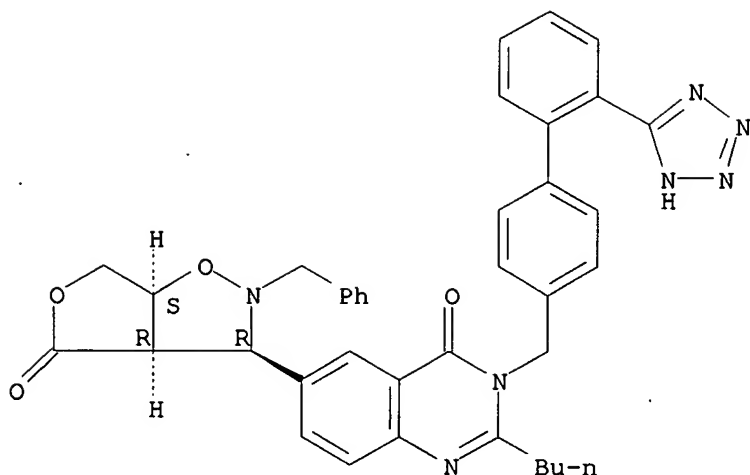
Relative stereochemistry.



RN 159040-15-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl) furo[3,4-d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\beta$,6 $\alpha\beta$)- (9CI) (CA INDEX NAME)

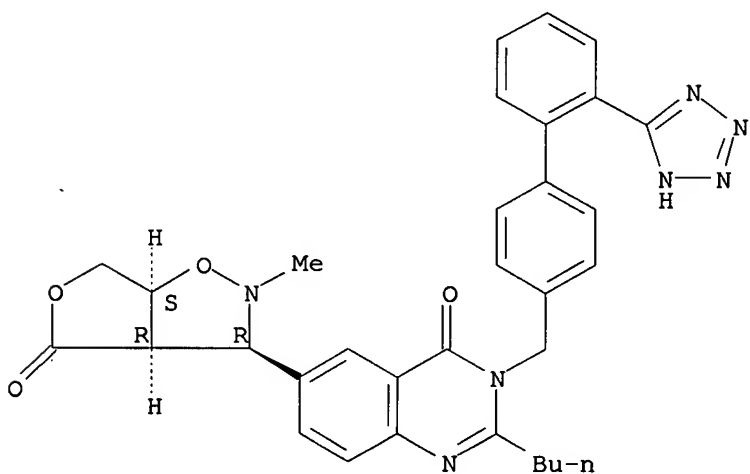
Relative stereochemistry.



RN 159168-90-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3αβ,6αβ)- (9CI) (CA INDEX NAME)

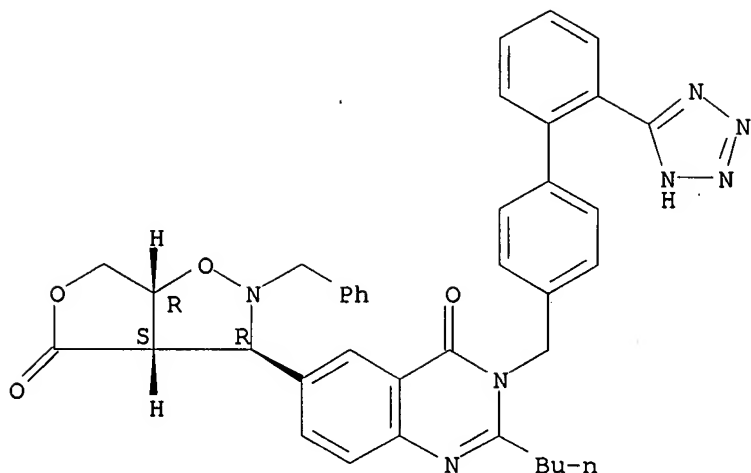
Relative stereochemistry.



RN 159168-91-9 ZCAPLUS

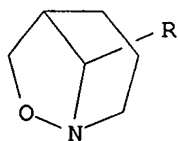
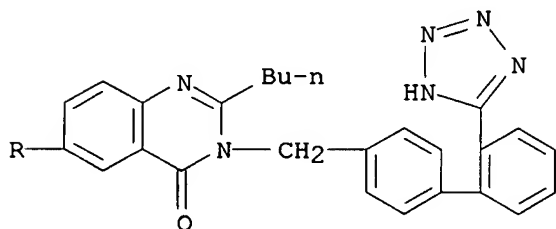
CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3αα,6αα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 160058-73-1 ZCAPLUS

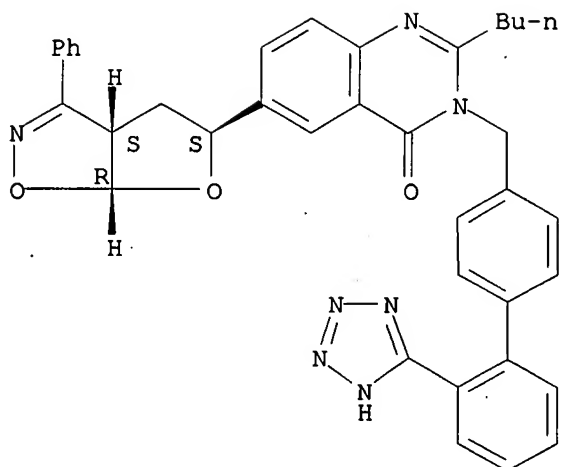
CN 4(3H)-Quinazolinone, 2-butyl-6-(7-oxa-1-azabicyclo[3.2.1]oct-8-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, anti- (9CI) (CA INDEX NAME)



RN 160058-75-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(3a,4,5,6a-tetrahydro-3-phenylfuro[3,2-d]isoxazol-5-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3aα,5α,6α)- (9CI) (CA INDEX NAME)

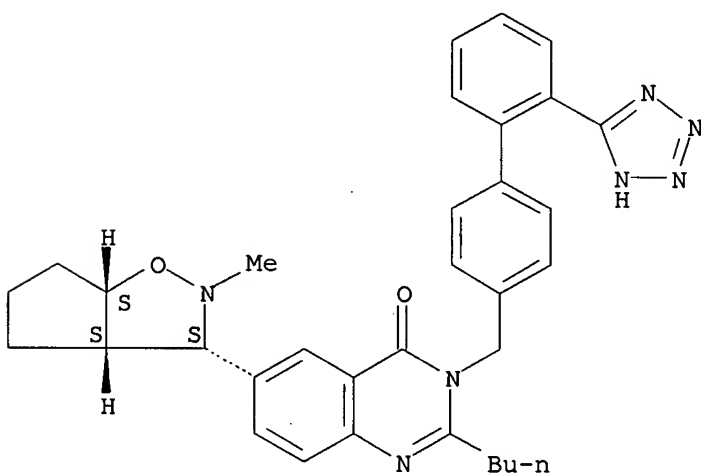
Relative stereochemistry.



RN 160167-90-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3aβ,6aβ)- (9CI) (CA INDEX NAME)

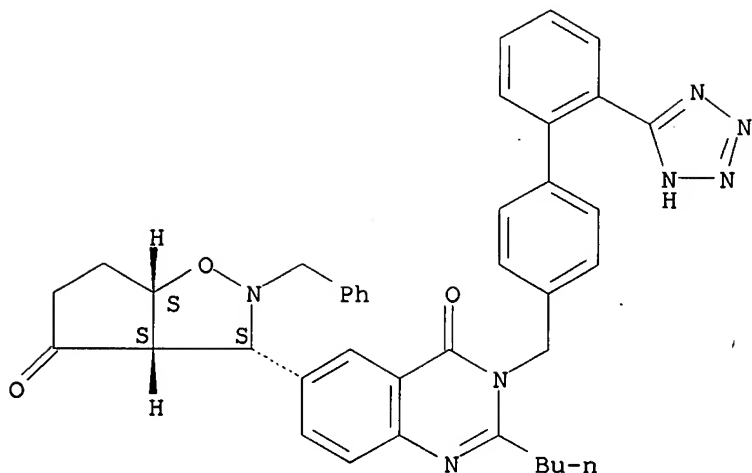
Relative stereochemistry.



RN 160167-92-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3aβ,6aβ)- (9CI) (CA INDEX NAME)

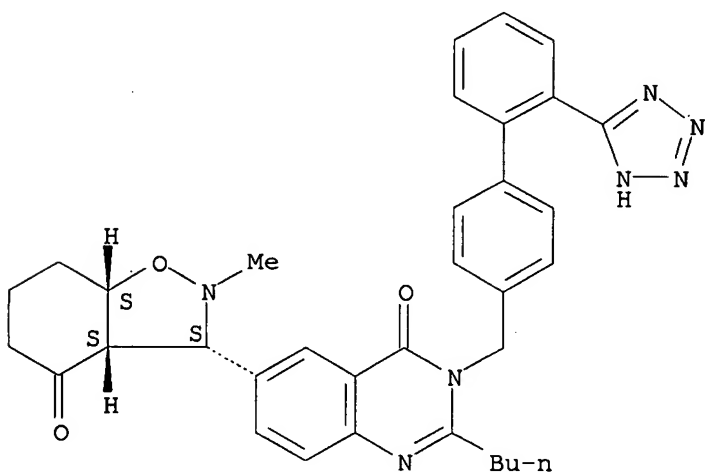
Relative stereochemistry.



RN 160167-93-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(octahydro-2-methyl-4-oxo-1,2-benzisoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

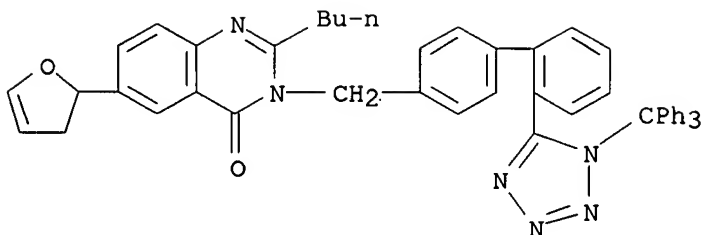


IT 158293-30-2 158293-40-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclyl-substituted quinazolinones as angiotensin II receptor antagonists)

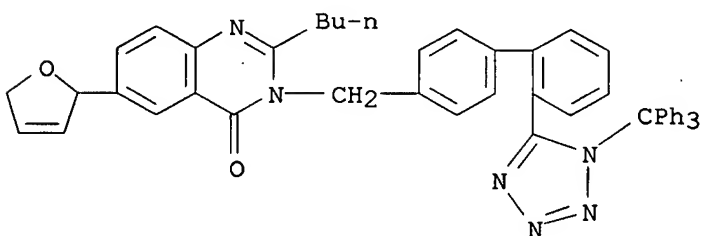
RN 158293-30-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2,3-dihydro-2-furanyl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



RN 158293-40-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2,5-dihydro-2-furanyl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



L4 ANSWER 59 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:32424 ZCAPLUS

DOCUMENT NUMBER: 122:56007

TITLE: 6-Isoxazolinyl and isoxazolidinyl substituted quinazolinones as angiotensin II receptor antagonists
AUTHOR(S): Levin, J. I.; Chan, P. S.; Coupet, J.; Bailey, T. K.; Vice, G.; Thibault, L.; Lai, F.; Venkatesan, A. M.; Cobuzzi, A.

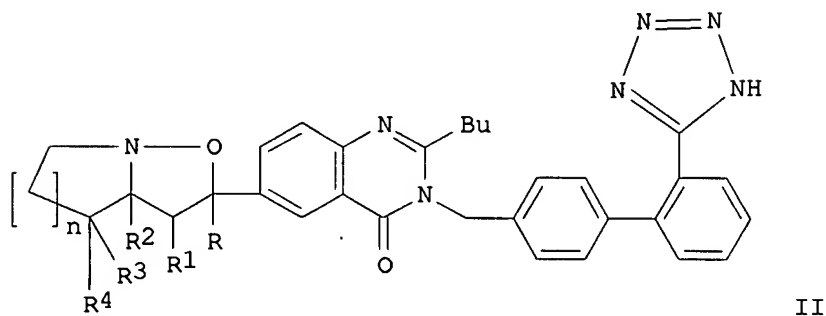
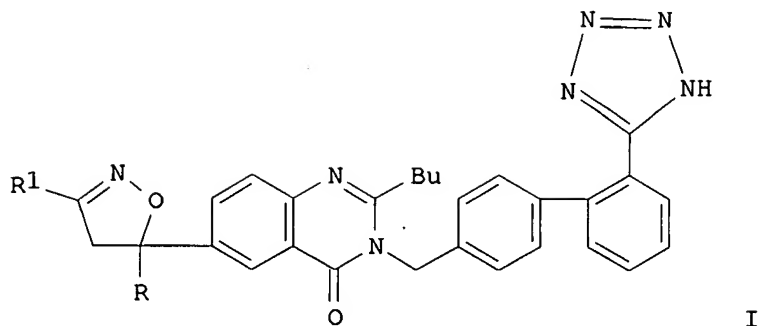
CORPORATE SOURCE: Lederle Lab., American Cyanamid Co., Pearl River, NY, 10965, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(14), 1703-8
CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



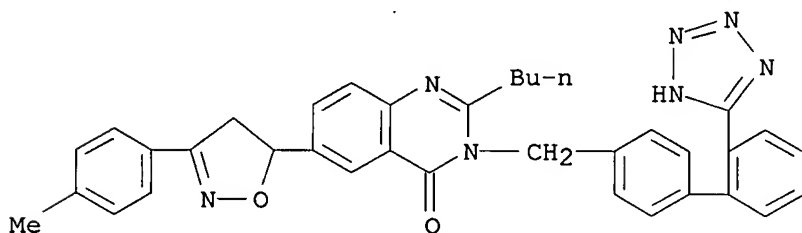
AB The preparation and biol. evaluation of 4(3H)-quinazolinones substituted at the 6-position with isoxazolidines and isoxazolidines is described. Example compds. are (isoxazolidinyl)quinazolinones I (R, R1 = substituent) and (pyrrolo[1,2-b]isoxazol-2-yl)quinazolinones and analogs II (R-R4 = substituent; n = integer).

IT 154749-04-9 154749-06-1 154749-08-3
 154749-11-8 155995-32-7 155995-34-9
 155995-35-0 155995-36-1 155995-40-7
 155995-41-8 155995-42-9 155995-43-0
 155995-44-1 155995-45-2 155995-47-4
 155995-53-2 159969-24-1 159969-25-2
 159969-27-4 159969-28-5 159969-30-9
 159969-31-0 159969-32-1 159969-33-2
 159969-34-3 160023-75-6 160023-76-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (angiotensin antagonist)

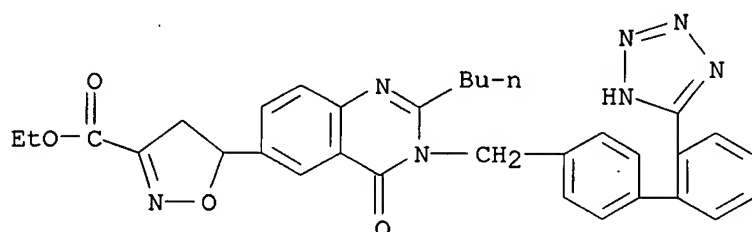
RN 154749-04-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methylphenyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
 (CA INDEX NAME)



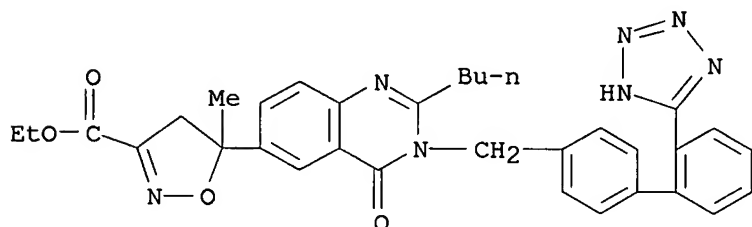
RN 154749-06-1 ZCAPLUS

CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-, ethyl ester (9CI) (CA INDEX NAME)



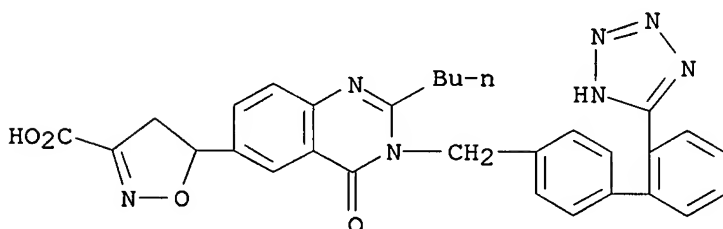
RN 154749-08-3 ZCAPLUS

CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 154749-11-8 ZCAPLUS

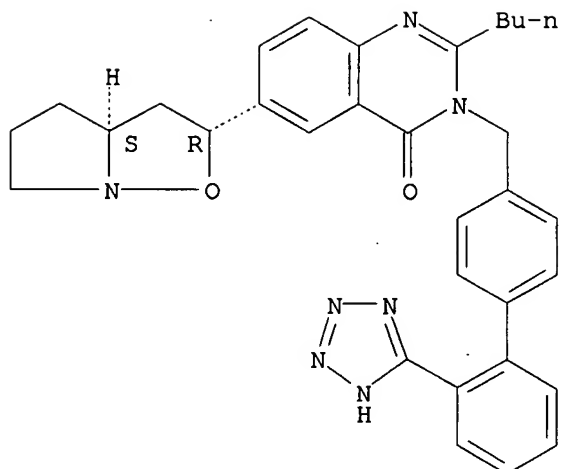
CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 155995-32-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

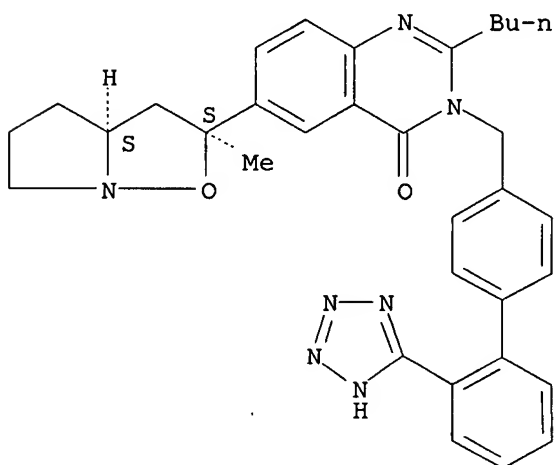
Relative stereochemistry.



RN 155995-34-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

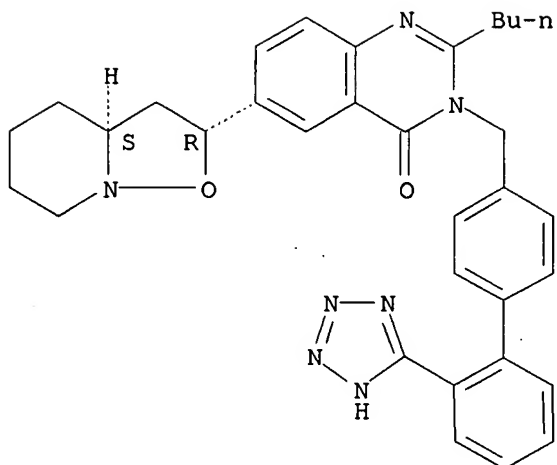
Relative stereochemistry.



RN 155995-35-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

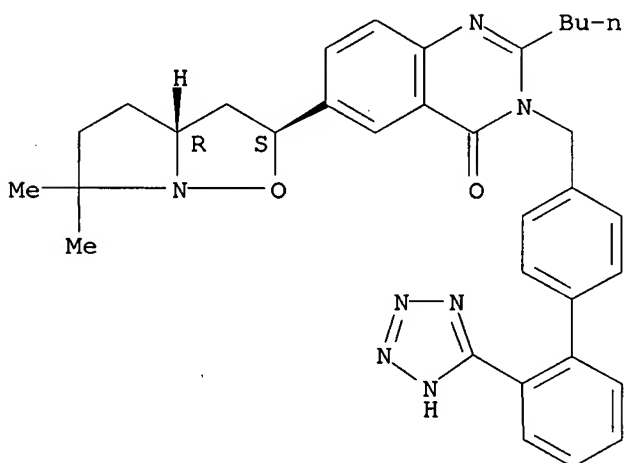
Relative stereochemistry.



RN 155995-36-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

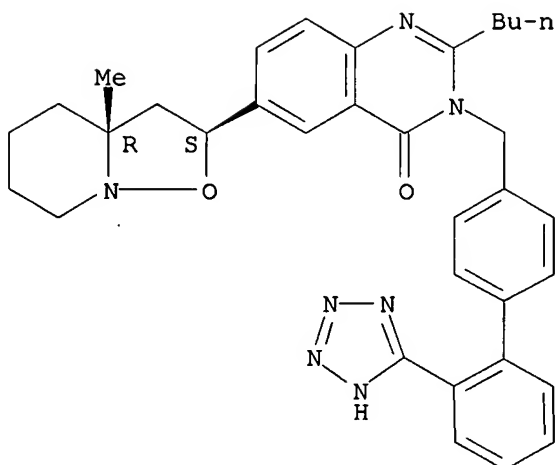
Relative stereochemistry.



RN 155995-40-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-3a-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

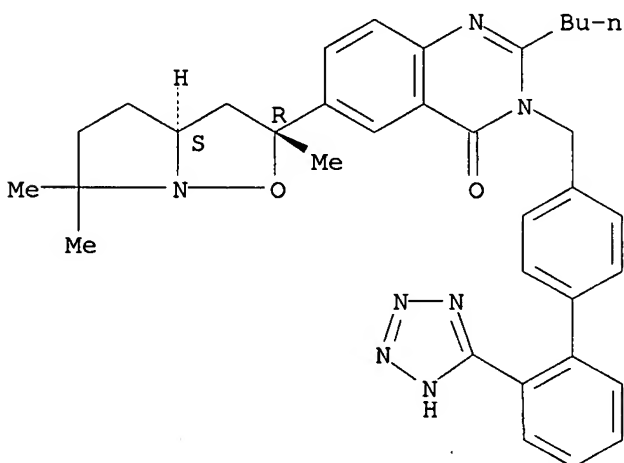
Relative stereochemistry.



RN 155995-41-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

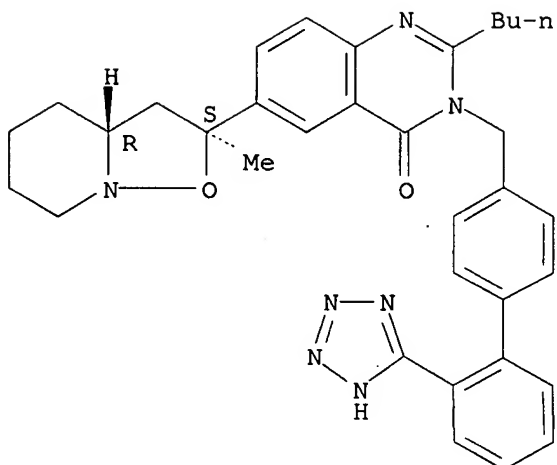
Relative stereochemistry.



RN 155995-42-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

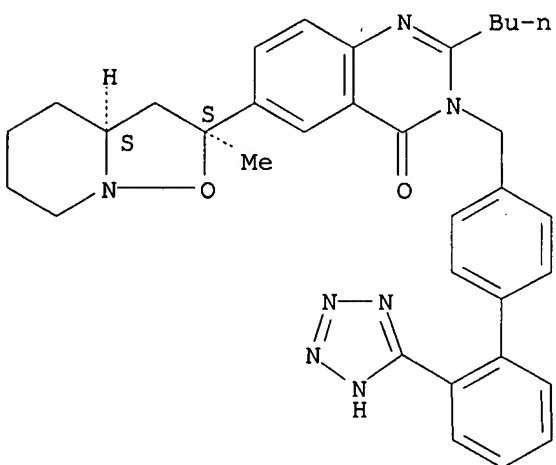
Relative stereochemistry.



RN 155995-43-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

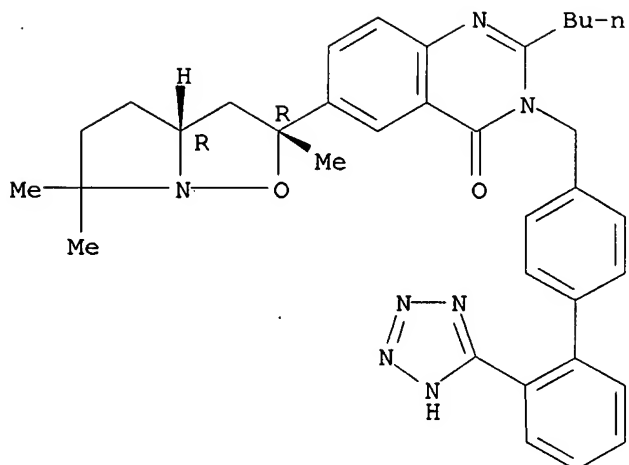
Relative stereochemistry.



RN 155995-44-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

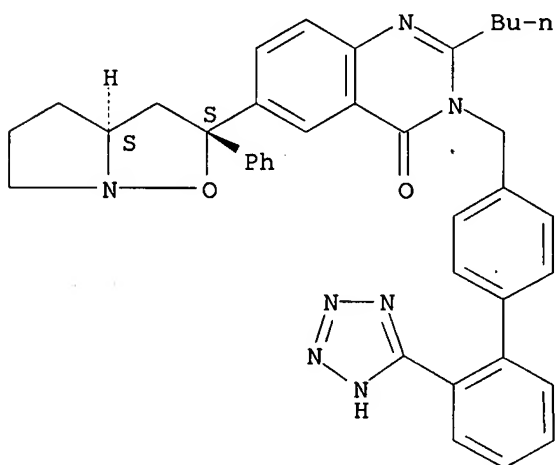
Relative stereochemistry.



RN 155995-45-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-phenylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI)
(CA INDEX NAME)

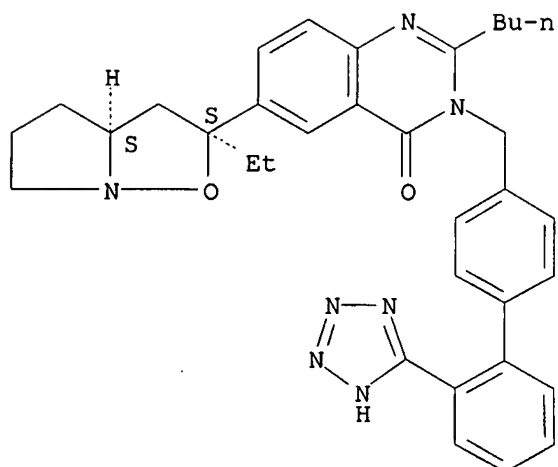
Relative stereochemistry.



RN 155995-47-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

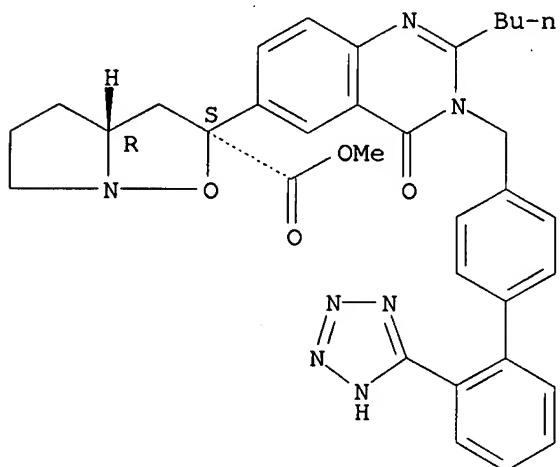
Relative stereochemistry.



RN 155995-53-2 ZCAPLUS

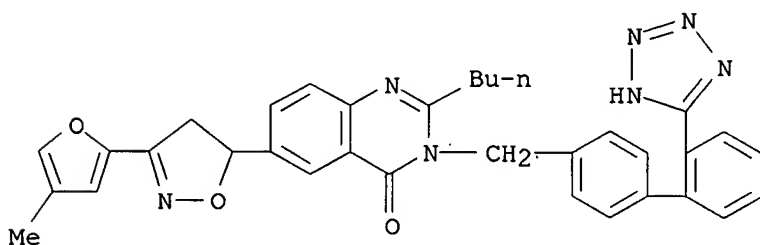
CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 159969-24-1 ZCAPLUS

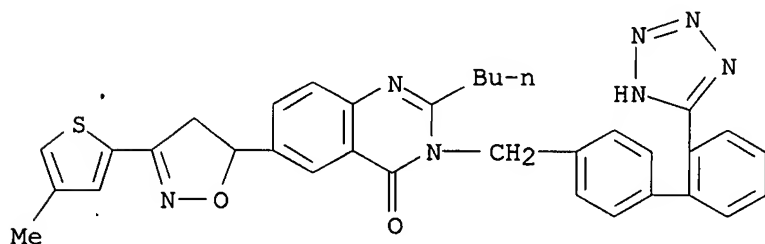
CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methyl-2-furanyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



10/ 530,897

RN 159969-25-2 ZCAPLUS

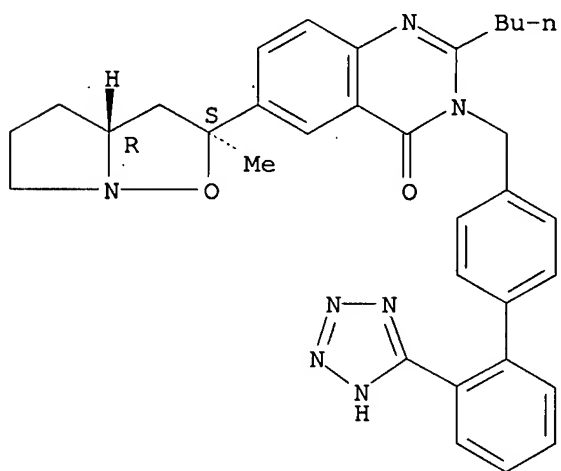
CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methyl-2-thienyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



RN 159969-27-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI)
(CA INDEX NAME)

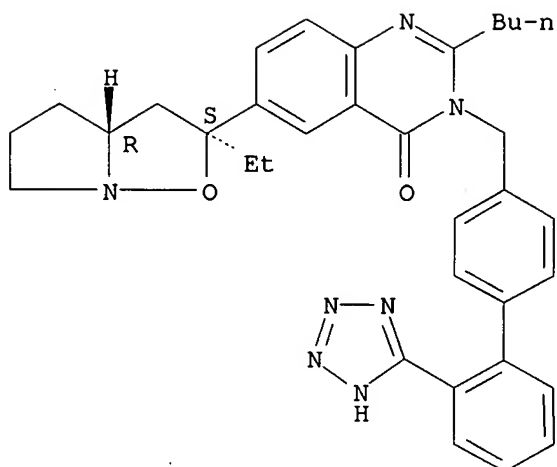
Relative stereochemistry.



RN 159969-28-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI)
(CA INDEX NAME)

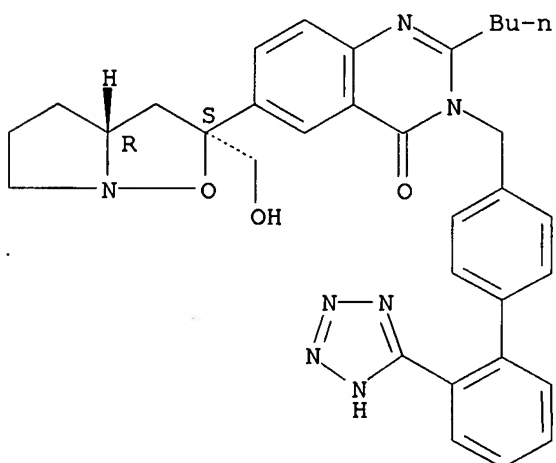
Relative stereochemistry.



RN 159969-30-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

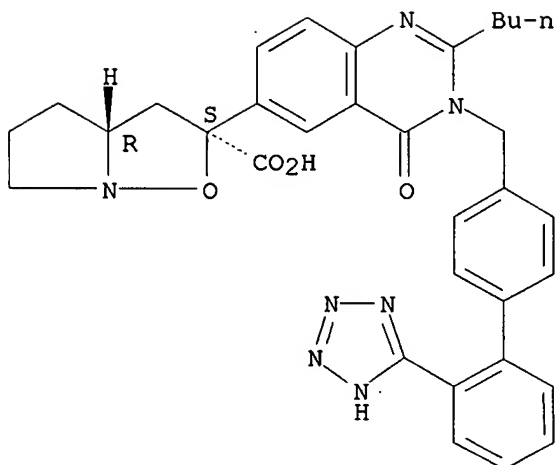
Relative stereochemistry.



RN 159969-31-0 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, trans- (9CI) (CA INDEX NAME)

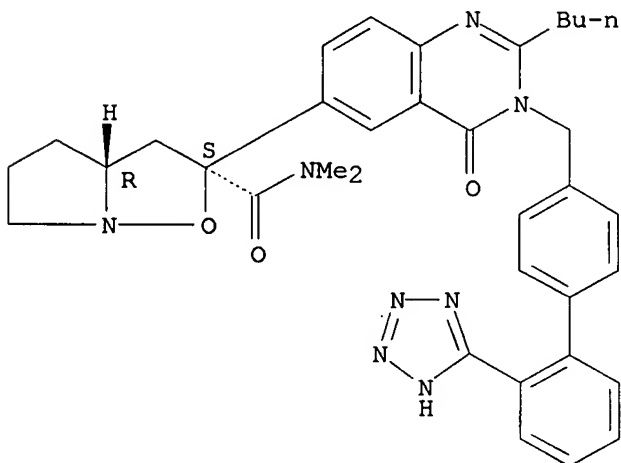
Relative stereochemistry.



RN 159969-32-1 ZCAPLUS

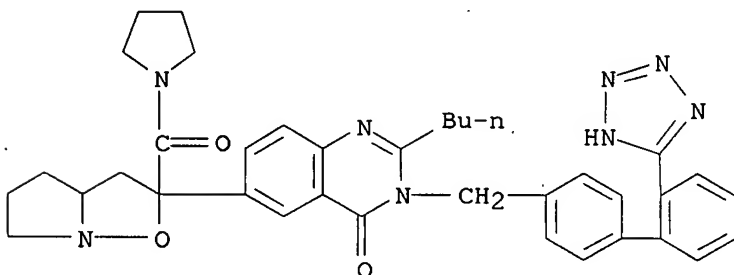
CN Pyrrolo[1,2-b]isoxazole-2-carboxamide, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



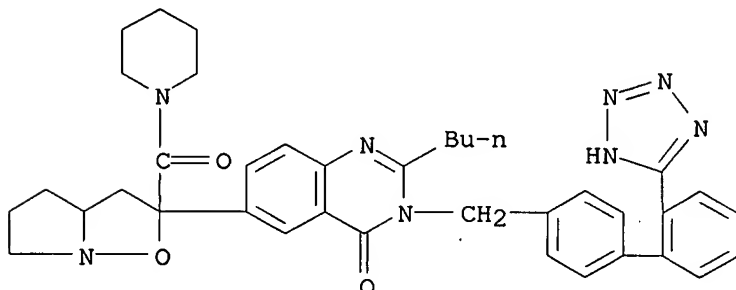
RN 159969-33-2 ZCAPLUS

CN Pyrrolidine, 1-[[2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydropyrrolo[1,2-b]isoxazol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)



RN 159969-34-3 ZCAPLUS

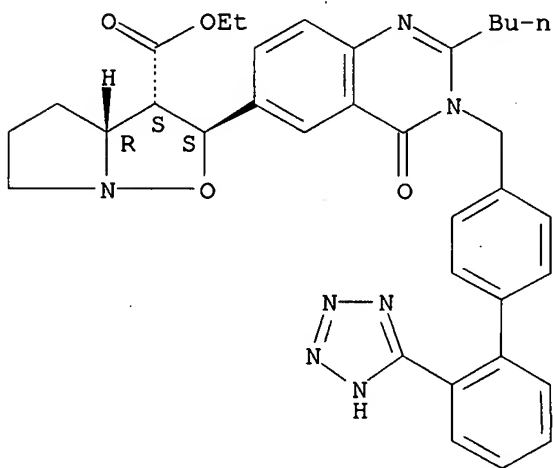
CN Piperidine, 1-[[[2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydropyrrolo[1,2-b]isoxazol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)



RN 160023-75-6 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, ethyl ester, (2 α ,3 β ,3 α)- (9CI) (CA INDEX NAME)

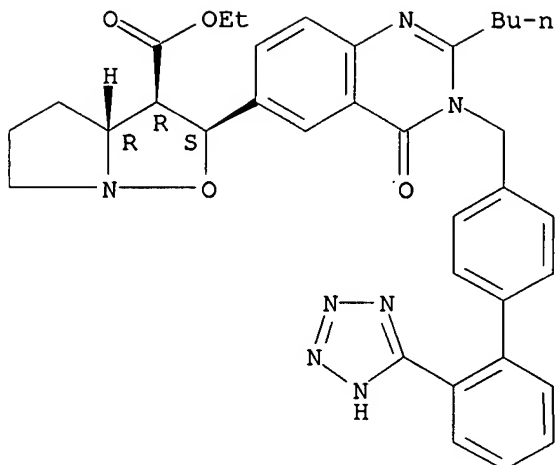
Relative stereochemistry.



RN 160023-76-7 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, ethyl ester, (2 α ,3 α ,3 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 60 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:5121 ZCAPLUS
 DOCUMENT NUMBER: 122:81387
 TITLE: Preparation of angiotensin II receptor blocking
 2,3,6-substituted quinazolinones
 INVENTOR(S): Venkatesan, Aranapakam M.; Levin, Jeremy I.
 PATENT ASSIGNEE(S): American Cyanamid Co., USA
 SOURCE: U.S., 16 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5294617	A	19940315	US 1993-52932	19930423
PRIORITY APPLN. INFO.:			US 1993-52932	19930423
OTHER SOURCE(S):	MARPAT	122:81387		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The preparation of title compds. I (R = 2-tetrazolyl; X = C3-5 alkyl, etc.; R6 = substituted heterocyclyl), which have activity as angiotensin II (AII) antagonists, is described. Thus, condensation of cis-2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-4(1H)-quinazolinone (preparation given) with 5-[4'-(bromomethyl)[1,1'-biphenyl]-2-yl]-1-(triphenylmethyl)-1H-tetrazole in the presence of K₂CO₃ in acetone followed by N-deprotection gave title compound II. IC₅₀(M) angiotensin II receptor binding of II was 4.3 x 10⁻⁸. Angiotensin II (AII) vasopressor response of compds. prepared was also given.

IT 155879-15-5P 155879-16-6P 155879-17-7P
 155879-18-8P

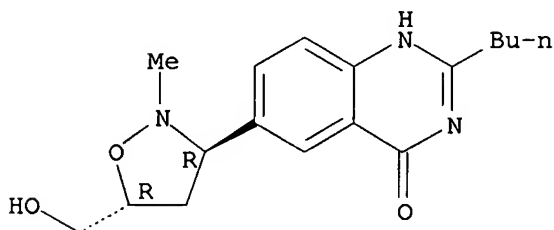
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of angiotensin II receptor antagonist)

10/ 530,897

RN 155879-15-5 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-, trans- (9CI) (CA INDEX NAME)

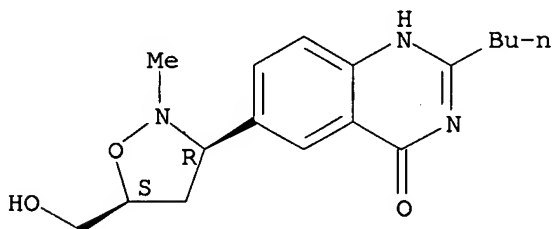
Relative stereochemistry.



RN 155879-16-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-, cis- (9CI) (CA INDEX NAME)

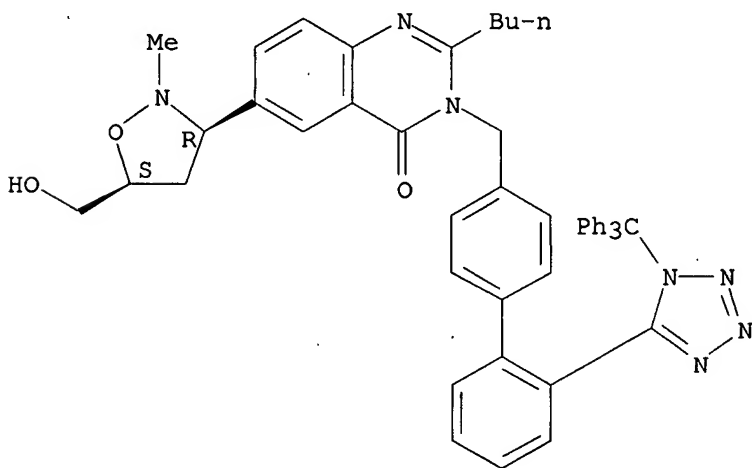
Relative stereochemistry.



RN 155879-17-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

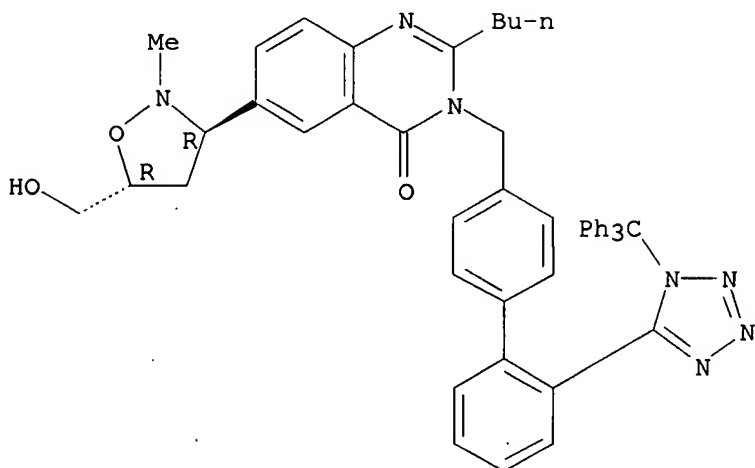
Relative stereochemistry.



RN 155879-18-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



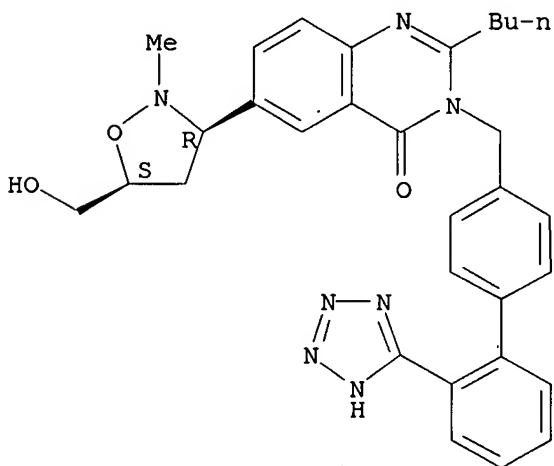
IT 155879-19-9P 155879-20-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as angiotensin II receptor antagonist)

RN 155879-19-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

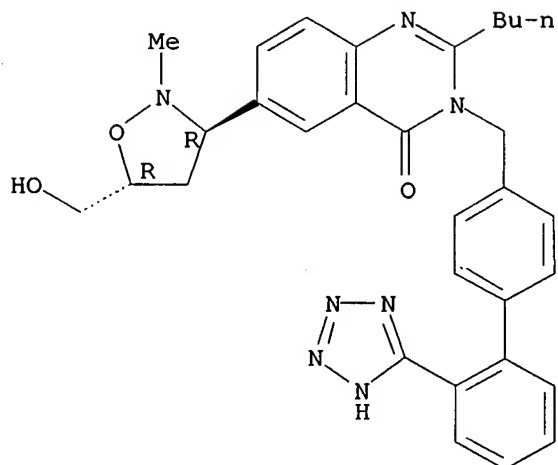
Relative stereochemistry.



RN 155879-20-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[5-(hydroxymethyl)-2-methyl-3-isoxazolidinyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 61 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:4668 ZCAPLUS
 DOCUMENT NUMBER: 122:10054
 TITLE: Preparation of (biphenylmethyl)quinazolinones as
 angiotensin II receptor blockers.
 INVENTOR(S): Levin, Jeremy I.; Venkatesan, Aranapakam M.
 PATENT ASSIGNEE(S): American Cyanamid Co., USA
 SOURCE: U.S., 31 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5292734	A	19940308	US 1993-52936	19930423
PRIORITY APPLN. INFO.:			US 1993-52936	19930423
OTHER SOURCE(S):	MARPAT	122:10054		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R = tetrazol-5-yl, CO₂H, NHSO₂CF₃; X = C₃₋₅ alkyl; R₆ = Q₁, Q₂, etc.; R₁, R₂, R₁₀, R₁₁, R₁₄ = H, (substituted) alkyl, Ph, pyridyl, thienyl, furyl, CO₂R₇, etc.; R₃ = H, alkyl, (substituted) Ph, pyridyl, thienyl, furyl, COR₅, CO₂R₇, etc.; R₄ = H, COR₅, CO₂R₇, alkyl, (substituted) Ph, PhCH₂, etc.; R₅, R₇ = H, alkyl; R₈ = H, alkyl, (substituted) Ph, COR₅; R₉ = H, alkyl, (substituted) Ph; A = (CR₁₁R₁₄)_m; X₁ = O, (CR₁₁R₁₄)_n, CO₂CONR₇; m = 2-5; n = 1-5; m+n ≤ 6], were prepared Thus, cis-2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-4(3H)-quinazolinone Na salt was heated with Zn in HOAc/H₂O at 65° for 5 h to give title compound II. II at 1 mg/kg i.v. in rats gave 93% inhibition of vasopressor response to angiotensin II at 0.05 µg/kg i.v.

IT 155995-56-5P

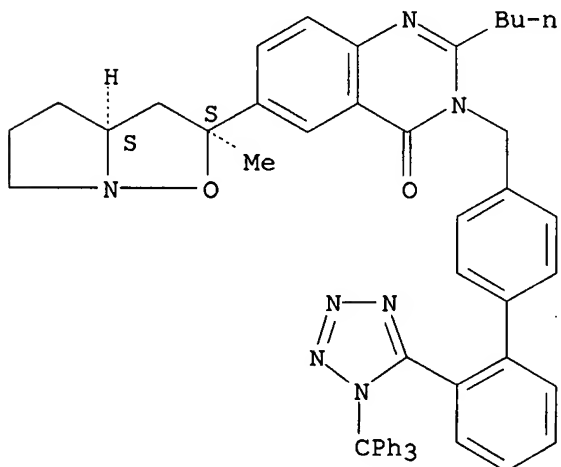
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

10/ 530,897

RN 155995-56-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



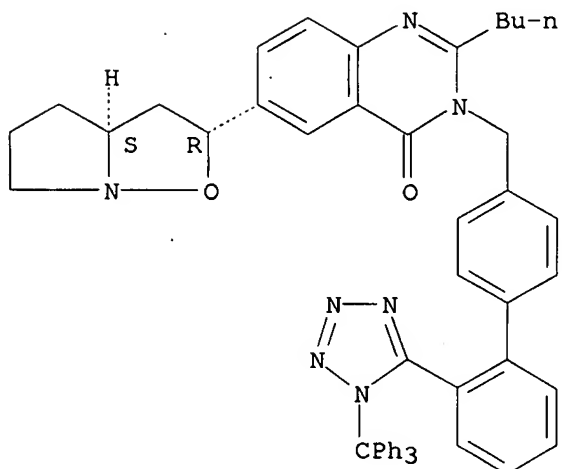
IT 155995-19-0P 155995-21-4P 155995-22-5P
155995-23-6P 155995-27-0P 155995-28-1P
155995-29-2P 155995-30-5P 155995-31-6P
155995-32-7P 155995-34-9P 155995-35-0P
155995-36-1P 155995-37-2P 155995-40-7P
155995-41-8P 155995-42-9P 155995-43-0P
155995-44-1P 155995-45-2P 155995-46-3P
155995-47-4P 155995-49-6P 155995-52-1P
155995-53-2P 155995-54-3P 155995-55-4P
157897-47-7P 159969-27-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as intermediate for angiotensin II antagonist)

RN 155995-19-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

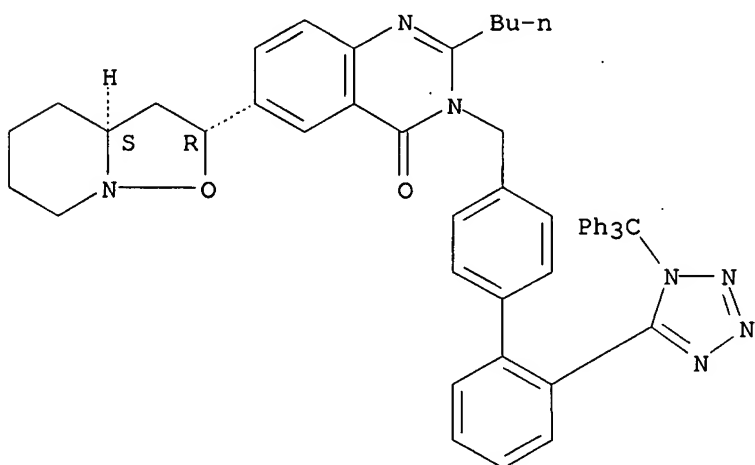
Relative stereochemistry.



RN 155995-21-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

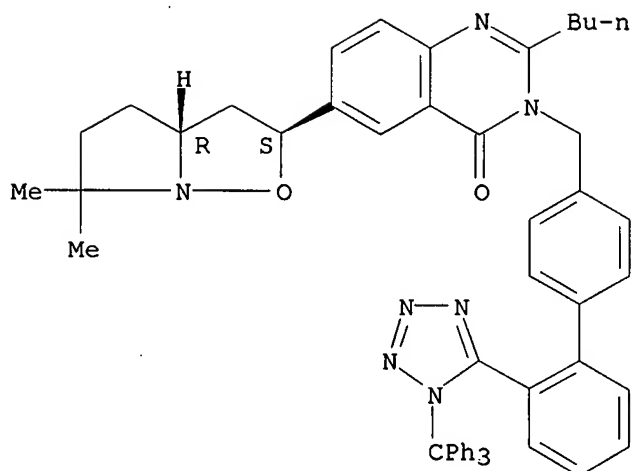
Relative stereochemistry.



RN 155995-22-5 ZCAPLUS

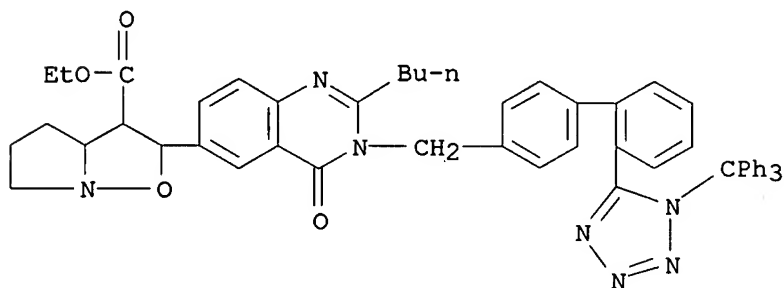
CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155995-23-6 ZCAPLUS

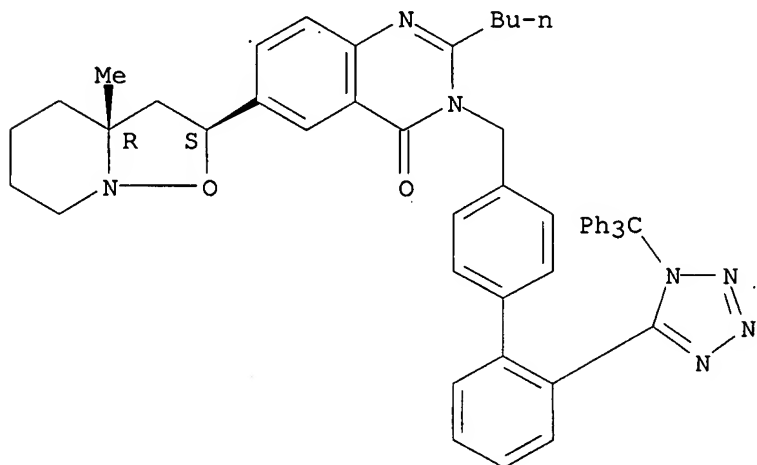
CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, ethyl ester (9CI) (CA INDEX NAME)



RN 155995-27-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-3a-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

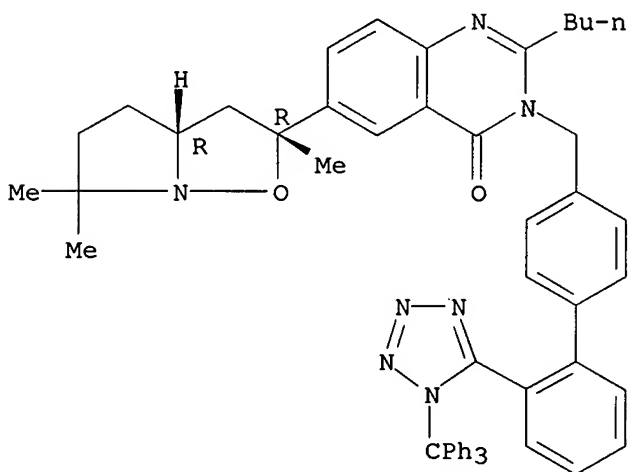
Relative stereochemistry.



RN 155995-28-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

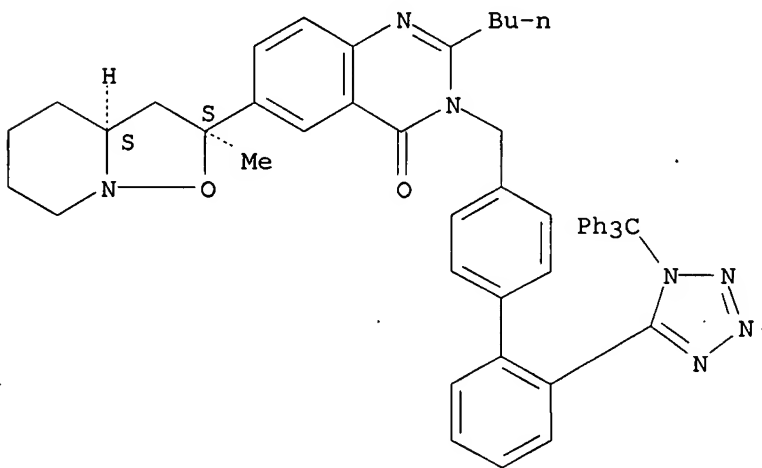
Relative stereochemistry.



RN 155995-29-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

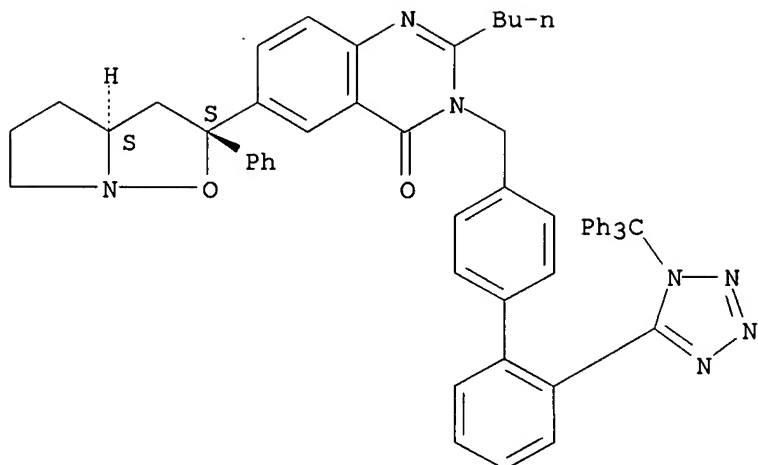
Relative stereochemistry.



RN 155995-30-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-phenylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

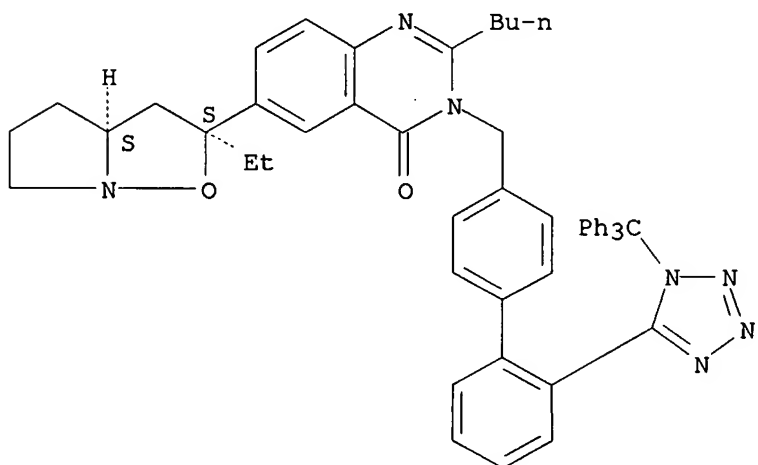
Relative stereochemistry.



RN 155995-31-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

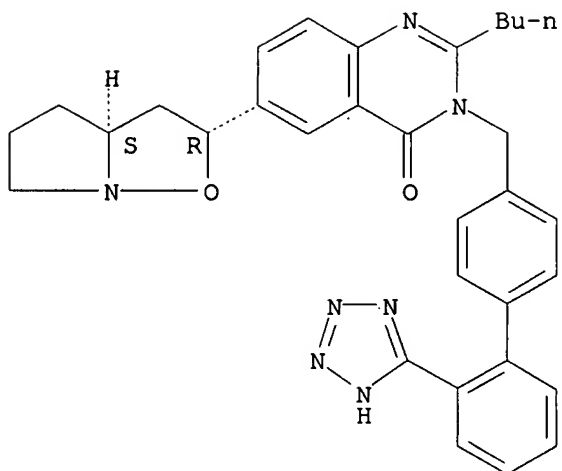
Relative stereochemistry.



RN 155995-32-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

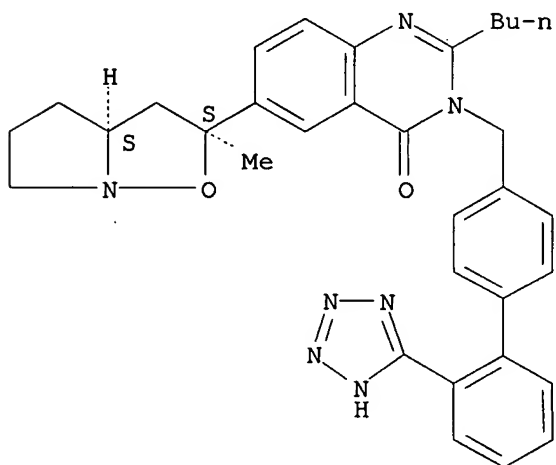
Relative stereochemistry.



RN 155995-34-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

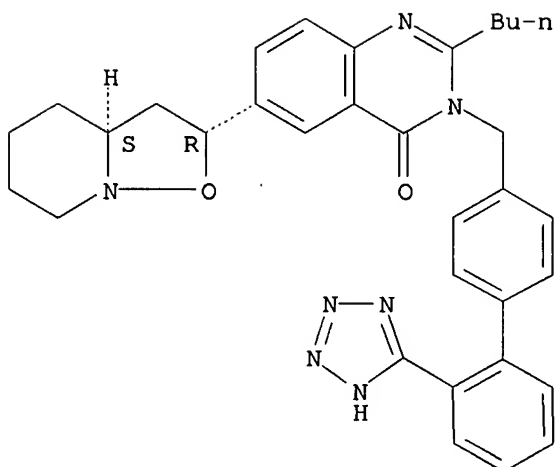
Relative stereochemistry.



RN 155995-35-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

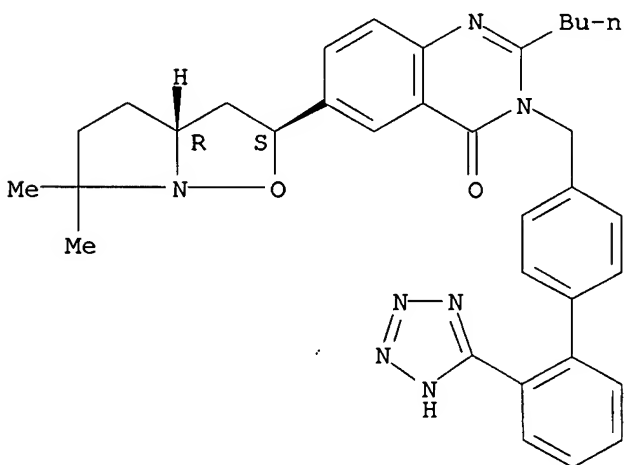
Relative stereochemistry.



RN 155995-36-1 ZCAPLUS

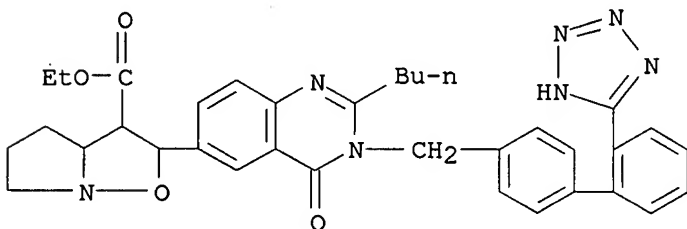
CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-6,6-dimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155995-37-2 ZCAPLUS

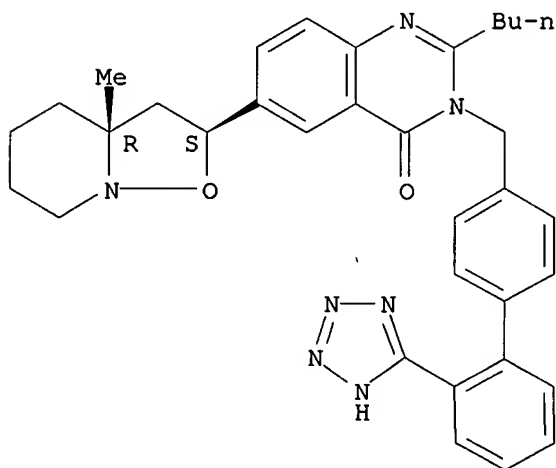
CN Pyrrolo[1,2-b]isoxazole-3-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, ethyl ester (9CI) (CA INDEX NAME)



RN 155995-40-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-3a-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

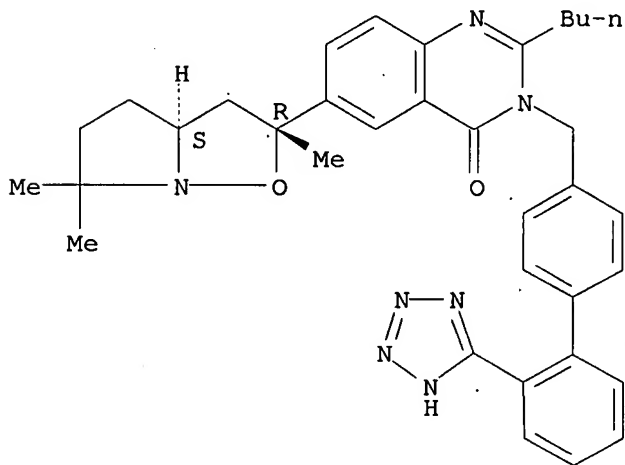
Relative stereochemistry.



RN 155995-41-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

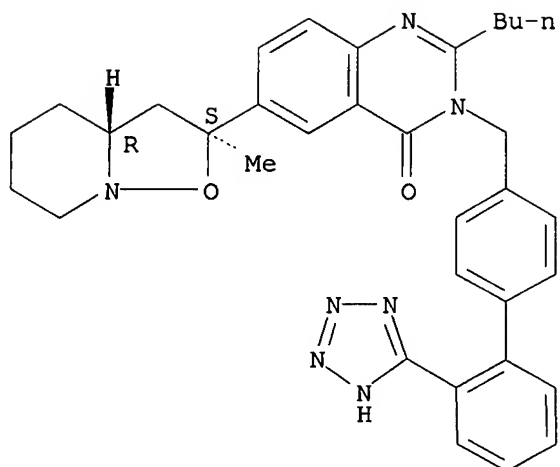
Relative stereochemistry.



RN 155995-42-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

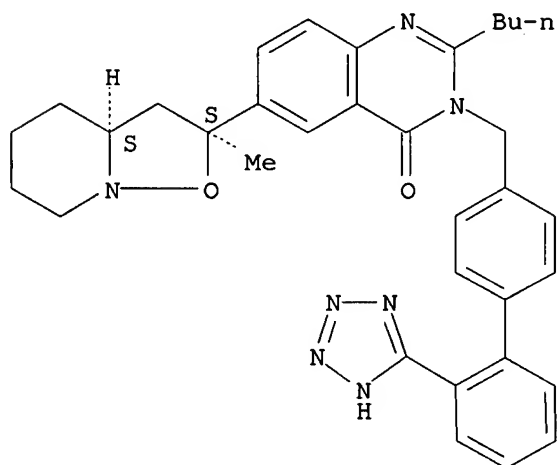
Relative stereochemistry.



RN 155995-43-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

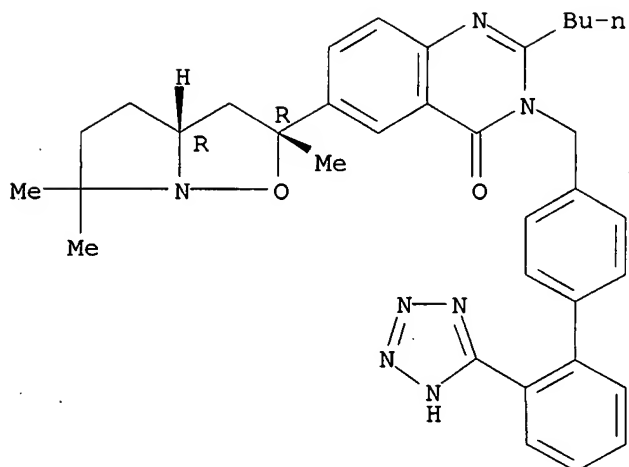
Relative stereochemistry.



RN 155995-44-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

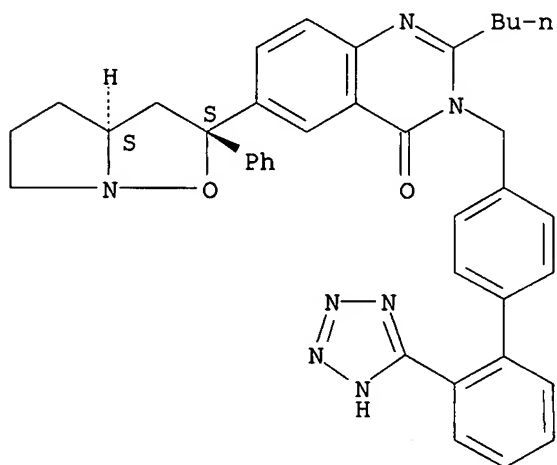
Relative stereochemistry.



RN 155995-45-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-phenylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI)
(CA INDEX NAME)

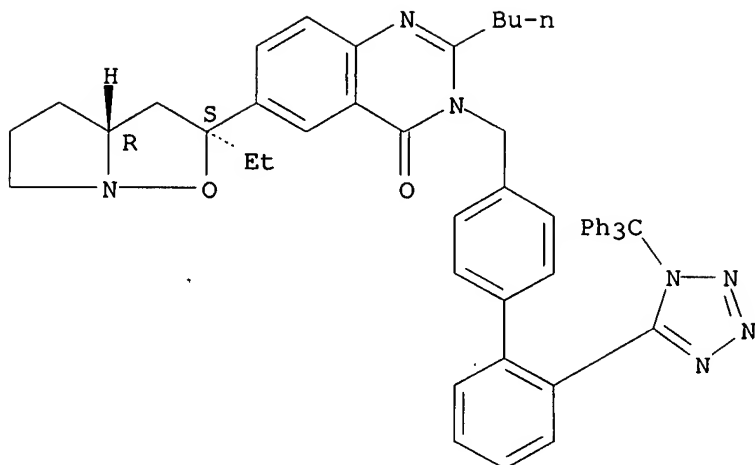
Relative stereochemistry.



RN 155995-46-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

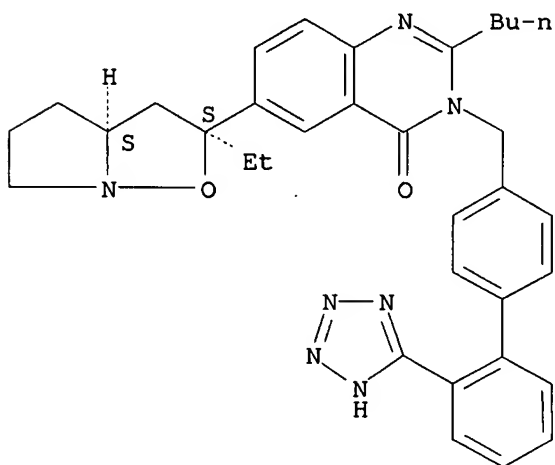
Relative stereochemistry.



RN 155995-47-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(2-ethylhexahydropyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI)
(CA INDEX NAME)

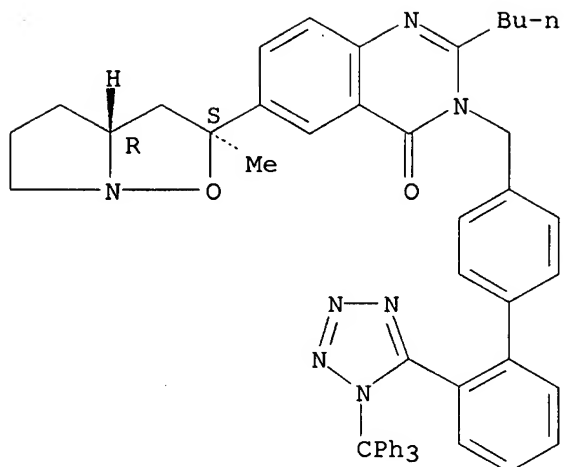
Relative stereochemistry.



RN 155995-49-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

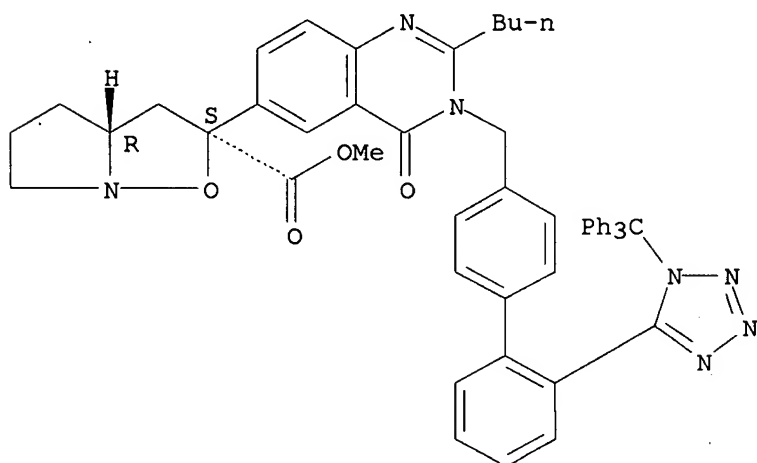
Relative stereochemistry.



RN 155995-52-1 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

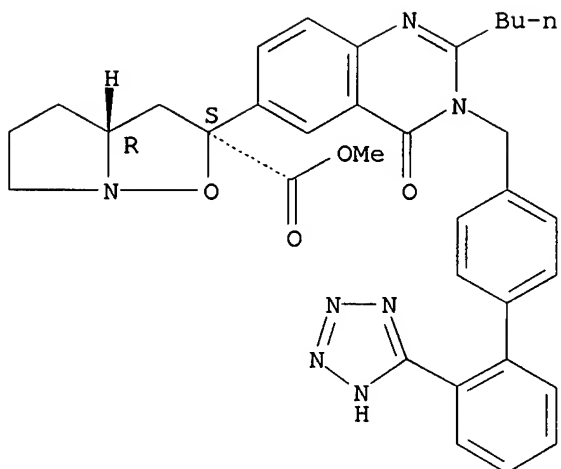
Relative stereochemistry.



RN 155995-53-2 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

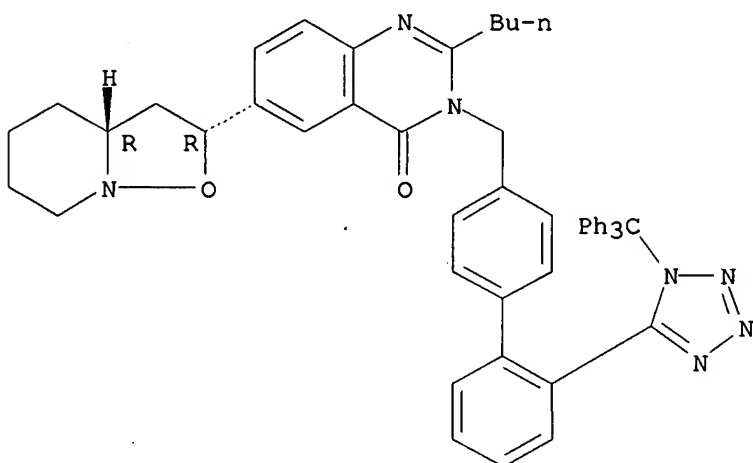
Relative stereochemistry.



RN 155995-54-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2H-isoxazolo[2,3-a]pyridin-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]-, trans- (9CI) (CA INDEX NAME)

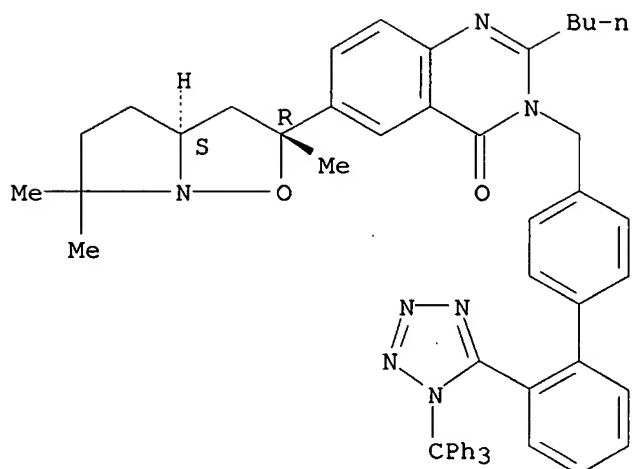
Relative stereochemistry.



RN 155995-55-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,6,6-trimethylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]-, cis- (9CI) (CA INDEX NAME)

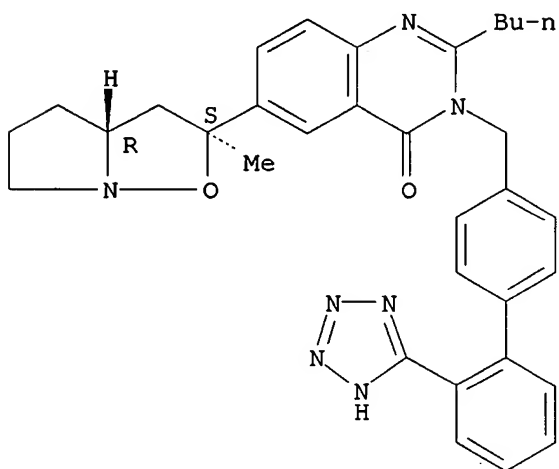
Relative stereochemistry.



RN 157897-47-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

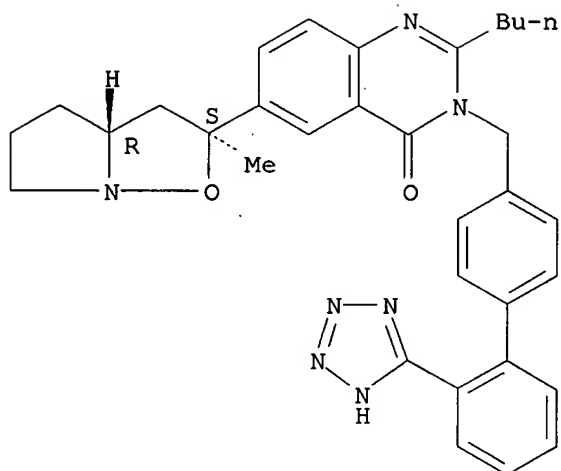


● Na

RN 159969-27-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 157897-47-7

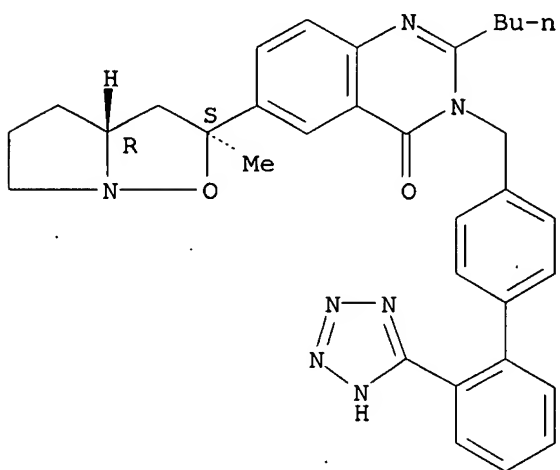
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of (biphenylmethyl)quinazolinone angiotensin II antagonist)

RN 157897-47-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Na

L4 ANSWER 62 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:700910 ZCAPLUS

DOCUMENT NUMBER: 121:300910

TITLE: Preparation of angiotensin II receptor blocking 2,3,6-substituted quinazolinones

INVENTOR(S): Venkatesan, Aranapakam M.; Levin, Jeremy I.

PATENT ASSIGNEE(S): American Cyanamid Co., USA

SOURCE: U.S., 33 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5294611	A	19940315	US 1993-52942	19930423
PRIORITY APPLN. INFO.:			US 1993-52942	19930423
OTHER SOURCE(S):	MARPAT	121:300910		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

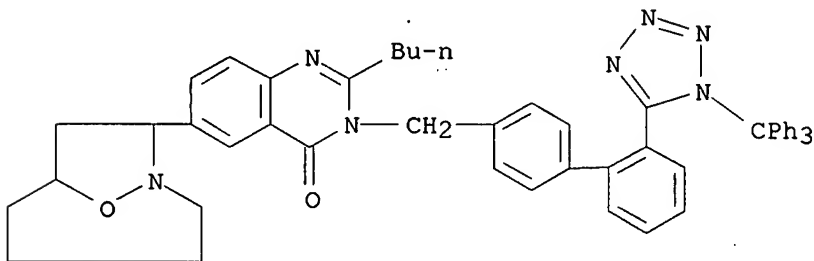
AB The preparation of title compds. I (R18 = 2-tetrazolyl, CO₂H, NHSO₂CF₃, etc.; X = C3-5 alkyl, etc.; R6 = substituted heterocyclyl), which have activity as angiotensin II (AII) antagonists, is described. Thus, condensation of 2-butyl-6-(hydroxymethyl)-4(1H)-quinazolinone (preparation given) with 5-[4'-(bromomethyl)[1,1'-biphenyl]-2-yl]-1-(triphenylmethyl)-1H-tetrazole in the presence of K₂CO₃ in acetone followed by oxidation, coupling with N-(5-hexenyl)hydroxylamine in Phme, and N-deprotection gave title compound II. IC₅₀(M) angiotensin II receptor binding of II was 4.2 x 10⁻⁸. Angiotensin II (AII) vasopressor response of compds. prepared was also given.

IT 159039-85-7P 159039-87-9P 159039-88-0P
 159039-92-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of angiotensin II receptor antagonist).

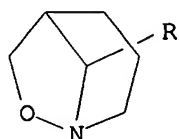
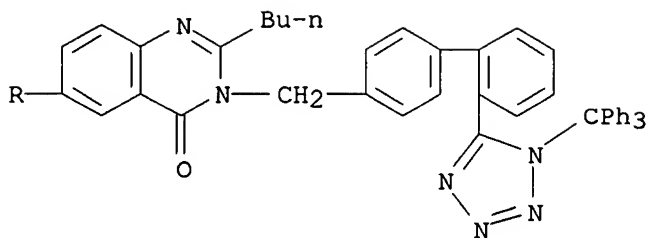
RN 159039-85-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(9-oxa-1-azabicyclo[4.2.1]non-8-yl)-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
 (CA INDEX NAME)



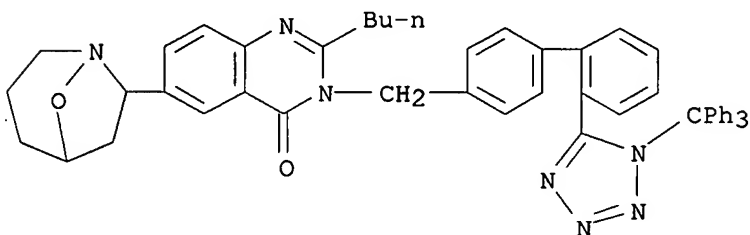
RN 159039-87-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(7-oxa-1-azabicyclo[3.2.1]oct-8-yl)-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
 (CA INDEX NAME)



RN 159039-88-0 ZCAPLUS

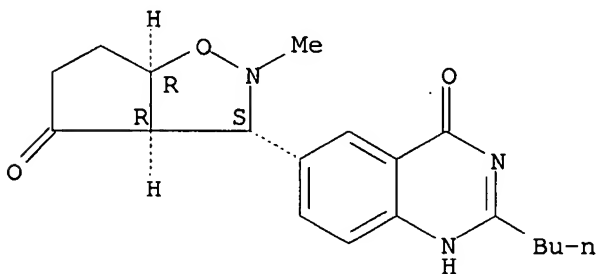
CN 4(3H)-Quinazolinone, 2-butyl-6-(8-oxa-1-azabicyclo[3.2.1]oct-7-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



RN 159039-92-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxo-2H-cyclopent[d]isoxazol-3-yl)-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 159039-86-8P 159039-89-1P 159039-92-6P
159039-94-8P 159039-96-0P 159039-97-1P
159039-98-2P 159039-99-3P 159040-00-3P
159040-01-4P 159040-03-6P 159040-05-8P
159040-06-9P 159040-07-0P 159040-08-1P
159040-09-2P 159040-10-5P 159040-13-8P
159040-14-9P 159040-15-0P 159168-86-2P

159168-87-3P 159168-88-4P 159168-89-5P

159168-90-8P 159168-91-9P 159168-92-0P

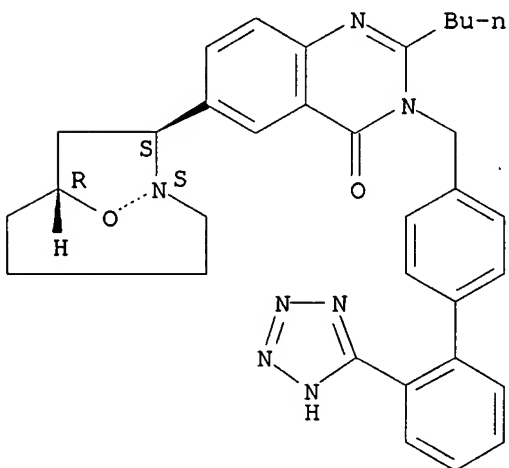
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as angiotensin II receptor antagonist)

RN 159039-86-8 ZCAPLUS

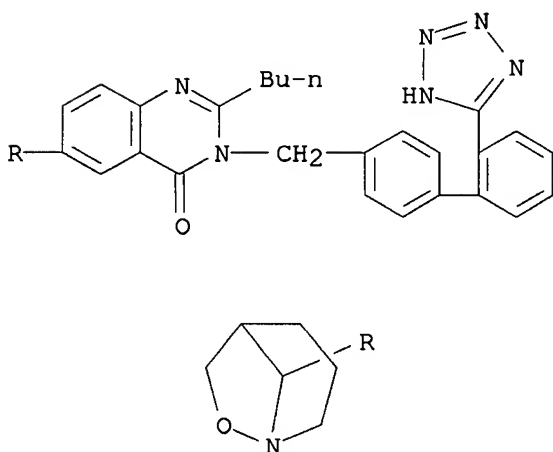
CN 4(3H)-Quinazolinone, 2-butyl-6-(9-oxa-1-azabicyclo[4.2.1]non-8-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 159039-89-1 ZCAPLUS

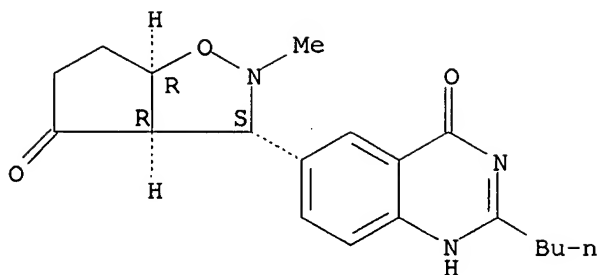
CN 4(3H)-Quinazolinone, 2-butyl-6-(7-oxa-1-azabicyclo[3.2.1]oct-8-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



RN 159039-92-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxo-2H-cyclopent[d]isoxazol-3-yl)-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

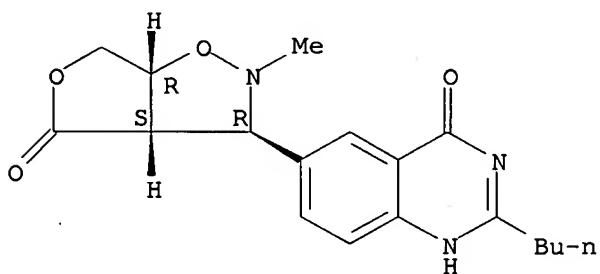
Relative stereochemistry.



RN 159039-94-8 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

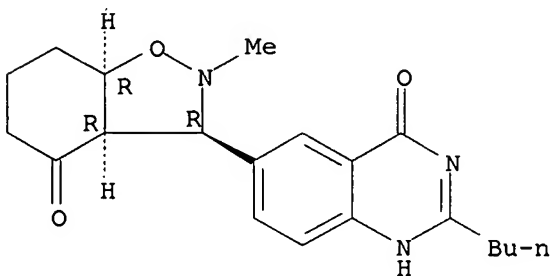
Relative stereochemistry.



RN 159039-96-0 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-(octahydro-2-methyl-4-oxo-1,2-benzisoxazol-3-yl)-, (3 α ,3 $\alpha\beta$,7 $\alpha\beta$)- (9CI) (CA INDEX NAME)

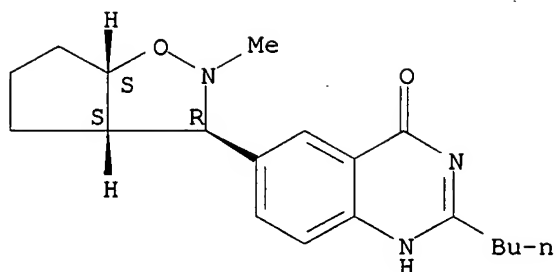
Relative stereochemistry.



RN 159039-97-1 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-cyclopent[d]isoxazol-3-yl)-, (3 α ,3 $\alpha\alpha$,6 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

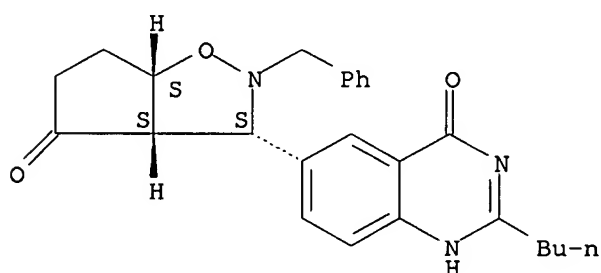
Relative stereochemistry.



RN 159039-98-2 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-, (3 α ,3a β ,6a β)- (9CI) (CA INDEX NAME)

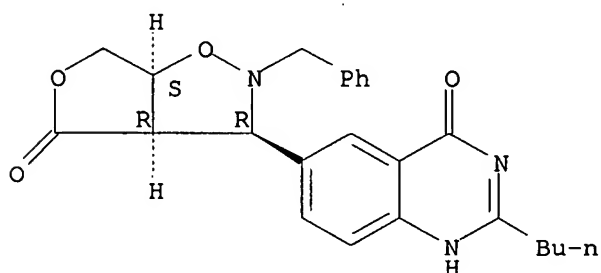
Relative stereochemistry.



RN 159039-99-3 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-, (3 α ,3a β ,6a β)- (9CI) (CA INDEX NAME)

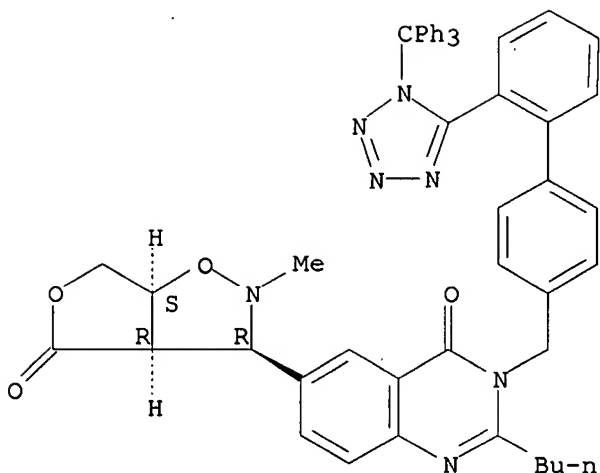
Relative stereochemistry.



RN 159040-00-3 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3a β ,6a β)- (9CI) (CA INDEX NAME)

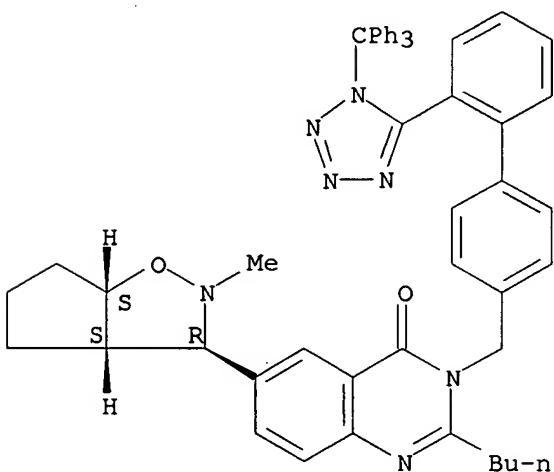
Relative stereochemistry.



RN 159040-01-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\alpha$,6 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

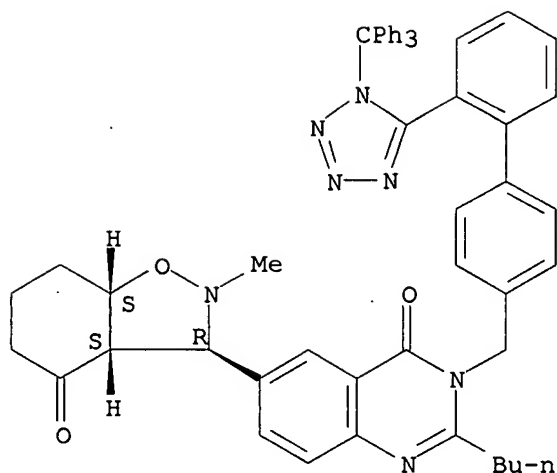
Relative stereochemistry.



RN 159040-03-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(octahydro-2-methyl-4-oxo-1,2-benzisoxazol-3-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\alpha$,7 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

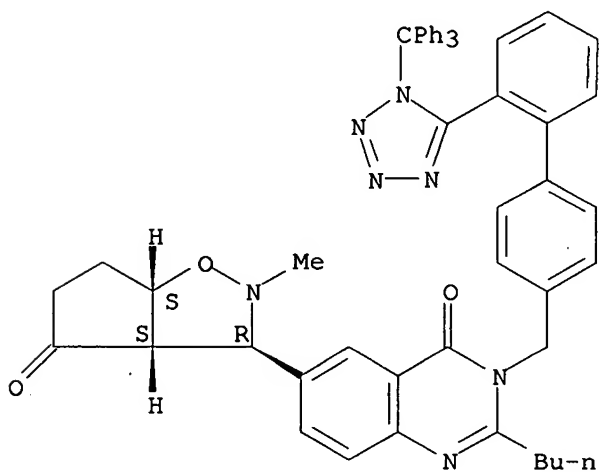
Relative stereochemistry.



RN 159040-05-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxo-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)- (9CI)
(CA INDEX NAME)

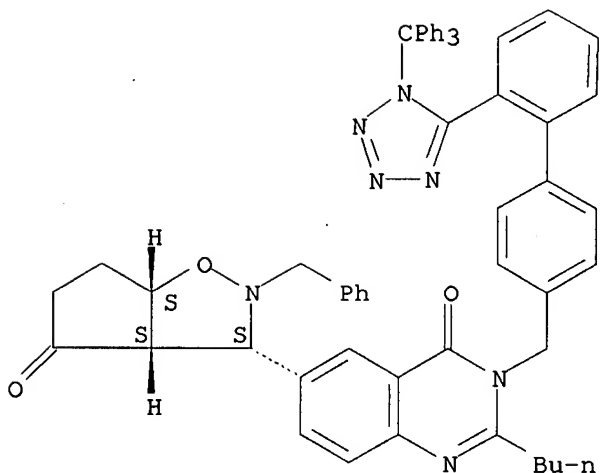
Relative stereochemistry.



RN 159040-06-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\beta$,6 $\alpha\beta$)- (9CI) (CA INDEX NAME)

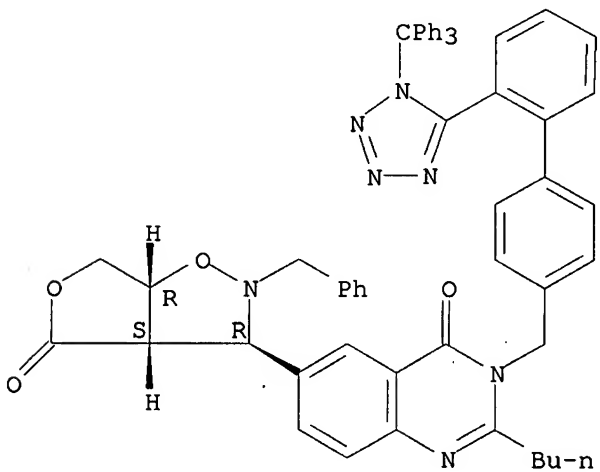
Relative stereochemistry.



RN 159040-07-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

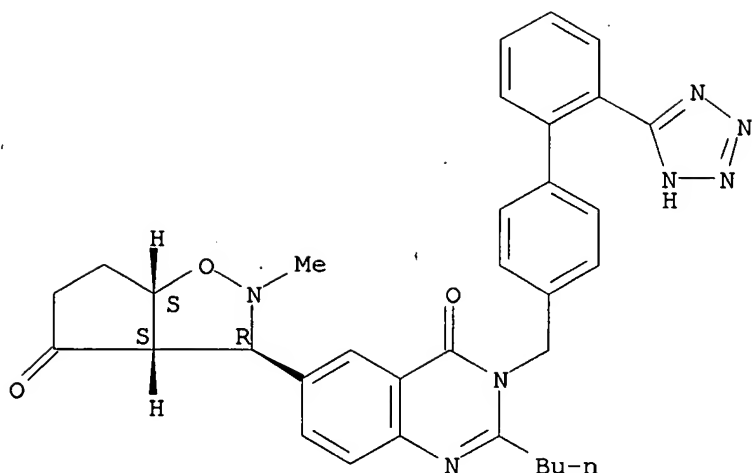
Relative stereochemistry.



RN 159040-08-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxo-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

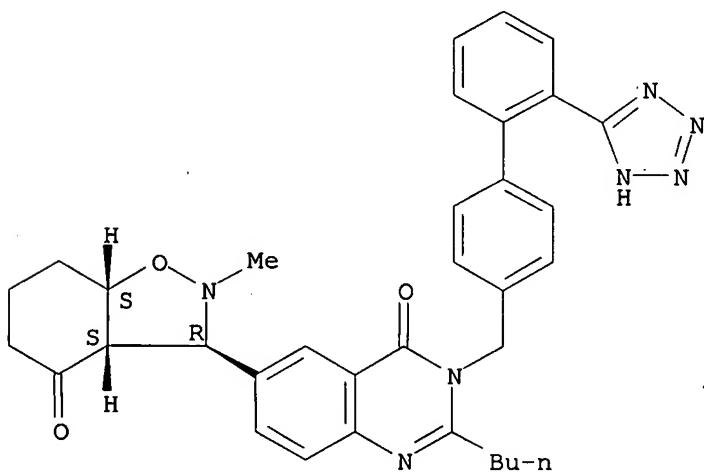
Relative stereochemistry.



RN 159040-09-2 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(octahydro-2-methyl-4-oxo-1,2-benzisoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3α,7α)- (9CI) (CA INDEX NAME)

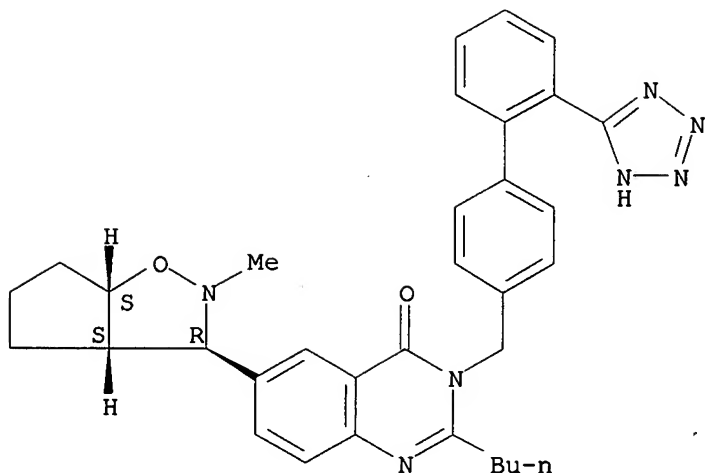
Relative stereochemistry.



RN 159040-10-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-2H-cyclopent[d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,3α,6α)- (9CI) (CA INDEX NAME)

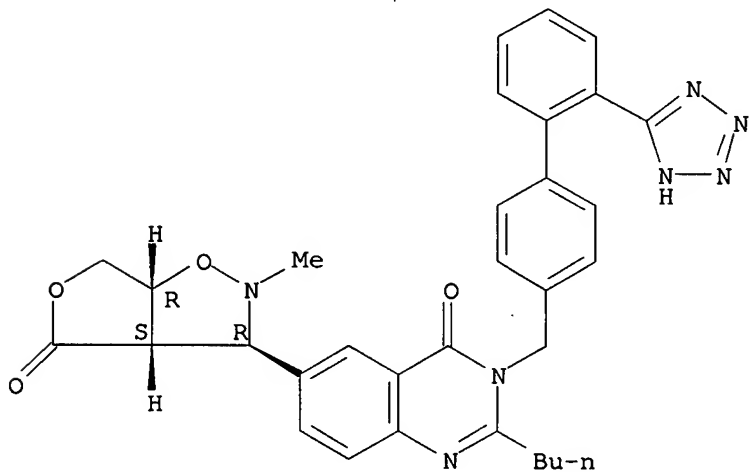
Relative stereochemistry.



RN 159040-13-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

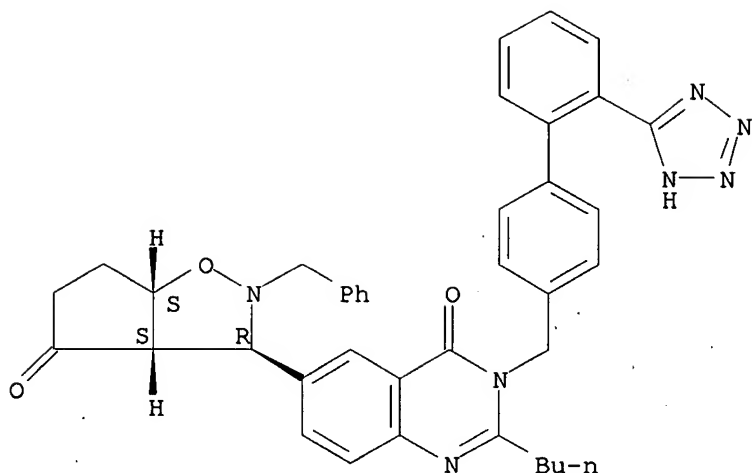
Relative stereochemistry.



RN 159040-14-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

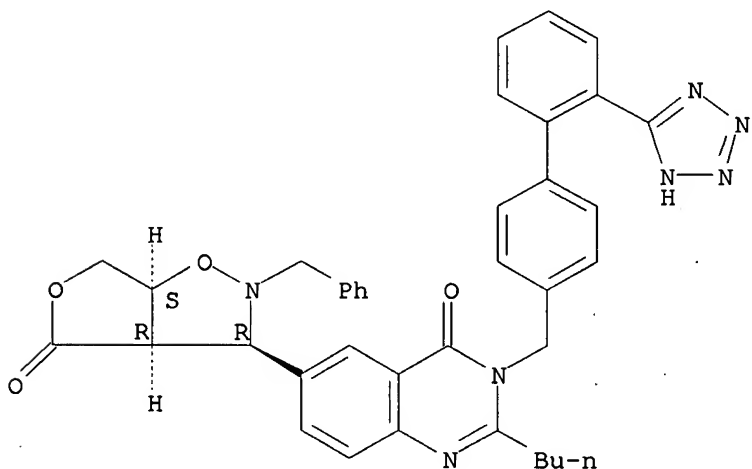
Relative stereochemistry.



RN 159040-15-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α β ,6 α β)-(9CI) (CA INDEX NAME)

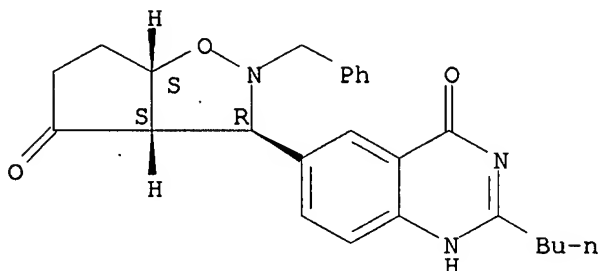
Relative stereochemistry.



RN 159168-86-2 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-, (3 α ,3 α α ,6 α α)-(9CI) (CA INDEX NAME)

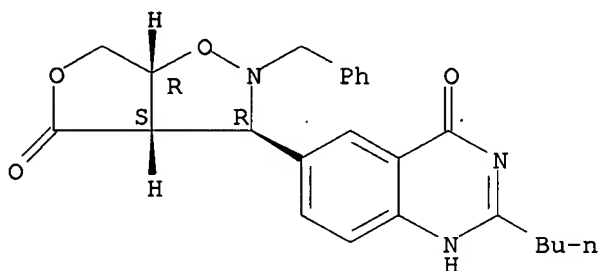
Relative stereochemistry.



RN 159168-87-3 ZCAPLUS

CN 4(1H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-, (3 α ,3 α ,6 α)- (9CI) (CA INDEX NAME)

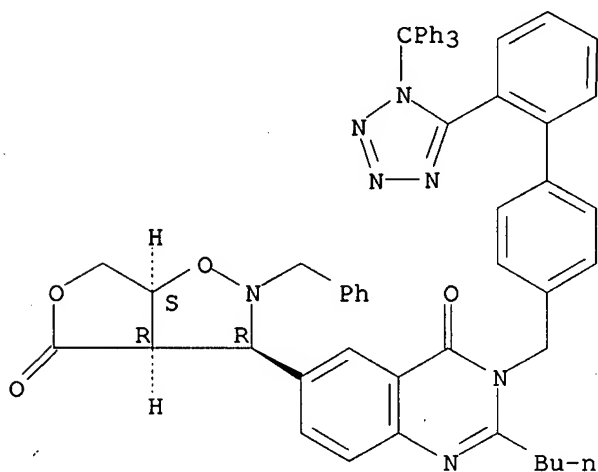
Relative stereochemistry.



RN 159168-88-4 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\beta$,6 $\alpha\beta$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

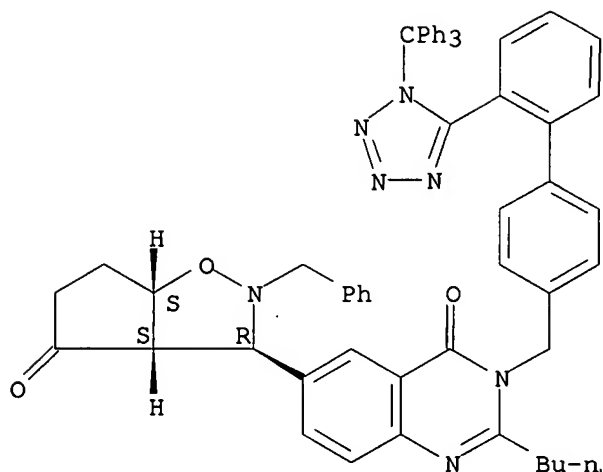


RN 159168-89-5 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)-2H-cyclopent[d]isoxazol-3-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)- (9CI)

(CA INDEX NAME)

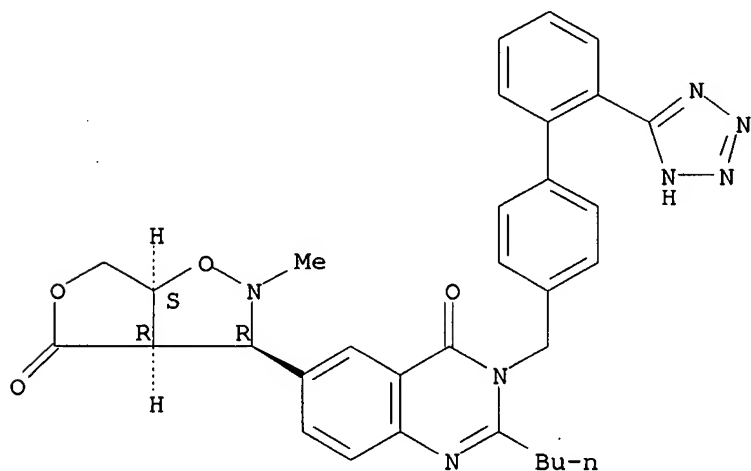
Relative stereochemistry.



RN 159168-90-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\beta$,6 $\alpha\beta$)- (9CI) (CA INDEX NAME)

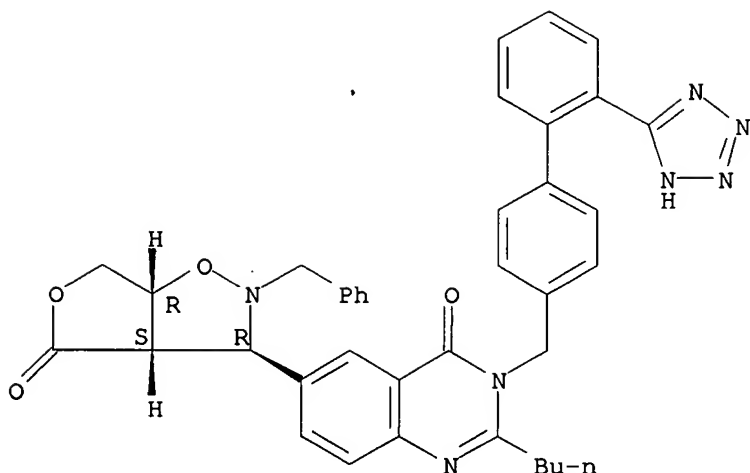
Relative stereochemistry.



RN 159168-91-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[hexahydro-4-oxo-2-(phenylmethyl)furo[3,4-d]isoxazol-3-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\alpha$,6 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

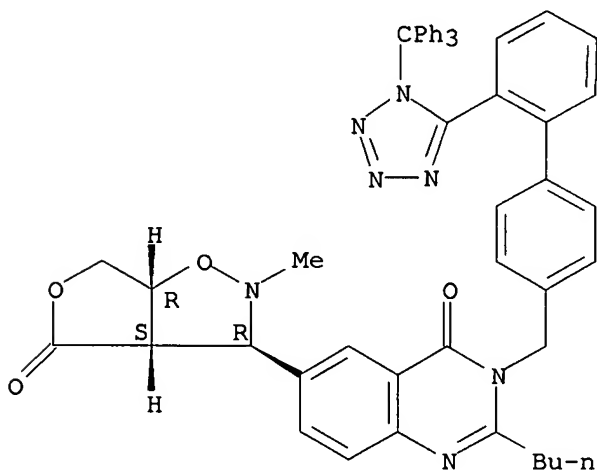
Relative stereochemistry.



RN 159168-92-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methyl-4-oxofuro[3,4-d]isoxazol-3-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 α ,6 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 63 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:630802 ZCAPLUS

DOCUMENT NUMBER: 121:230802

TITLE: Angiotensin II receptor blocking 2,3,6-substituted quinazolinones

INVENTOR(S): Levin, Jeremy I.; Venkatesan, Aranapakam M.

PATENT ASSIGNEE(S): American Cyanamid Co., USA

SOURCE: U.S., 15 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

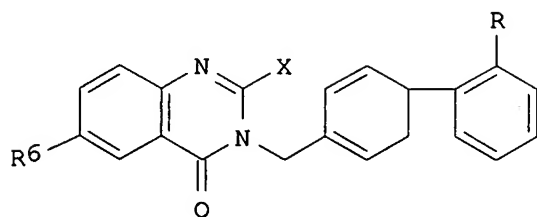
PATENT NO.

KIND DATE

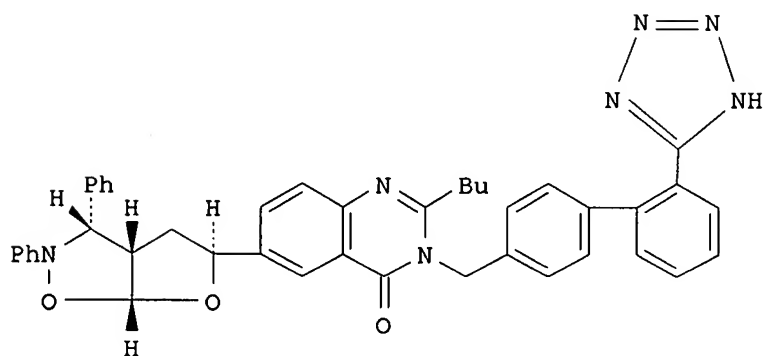
APPLICATION NO.

DATE

US 5281604	A	19940125	US 1993-52944	19930423
PRIORITY APPLN. INFO.:			US 1993-52944	19930423
OTHER SOURCE(S):	MARPAT 121:230802			
GI				



I



II

AB The invention provides novel 2,3,6 substituted quinazolinones of the formula I (tetrazolyl; X = alkyl; R6 = heterocyclyl); I activity as angiotensin II (AII) antagonists. I are claimed for the treatment of congestive heart failure and as antihypertensives. An example compound is the (2,3-diphenylfuro[2,3-d]isoxazolyl)[[(tetrazolyl)biphenyl]methyl]quinazolinone II.

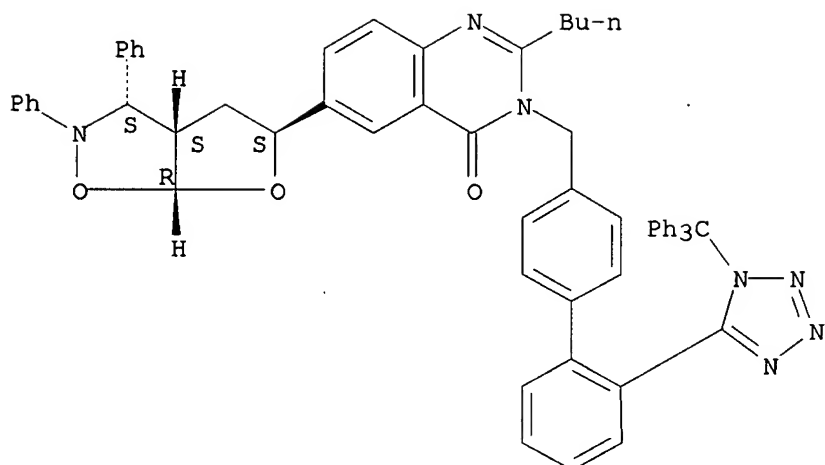
IT 158293-34-6P 158293-36-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 158293-34-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,3-diphenylfuro[3,2-d]isoxazol-5-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3 α ,3 $\alpha\beta$,5 β ,6 $\alpha\beta$)-(9CI) (CA INDEX NAME)

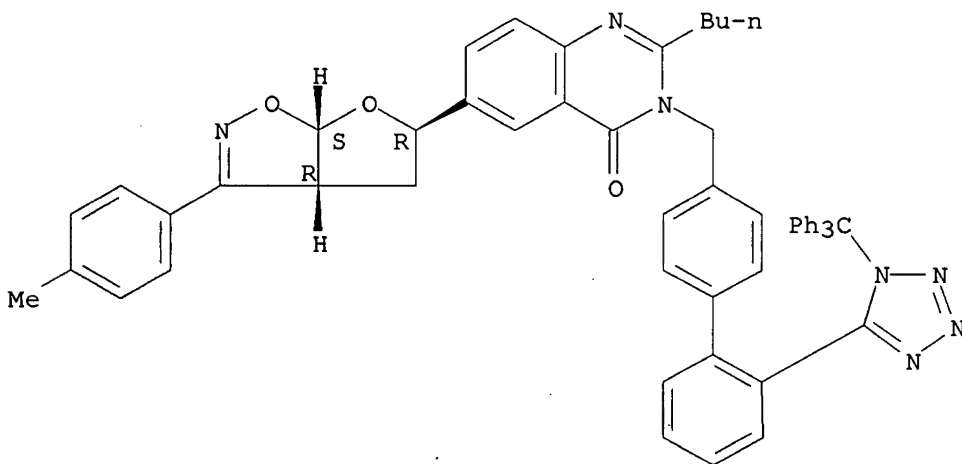
Relative stereochemistry.



RN 158293-36-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[3a,4,5,6a-tetrahydro-3-(4-methylphenyl)furo[3,2-d]isoxazol-5-yl]-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, (3a α ,5 α ,6a α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



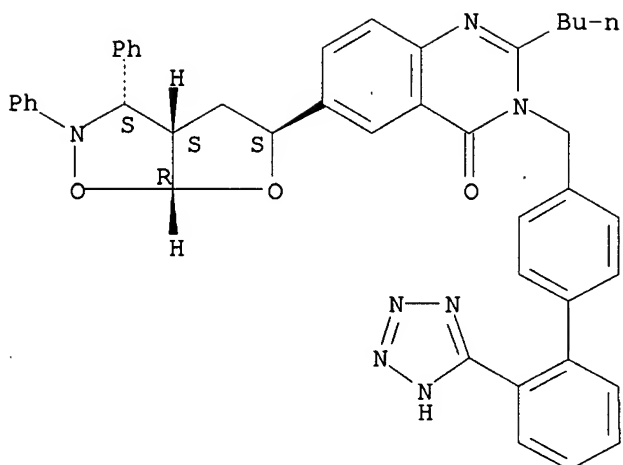
IT 158293-35-7P 158293-37-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as angiotensin antagonist antihypertensive)

RN 158293-35-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2,3-diphenylfuro[3,2-d]isoxazol-5-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3a α ,3a β ,5 β ,6a β)-(9CI) (CA INDEX NAME)

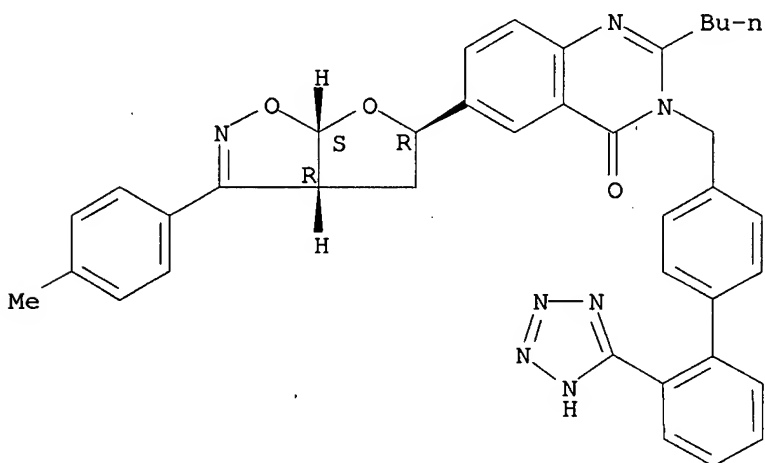
Relative stereochemistry.



RN 158293-37-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[3a,4,5,6a-tetrahydro-3-(4-methylphenyl)furo[3,2-d]isoxazol-5-yl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (3α,5α,6α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



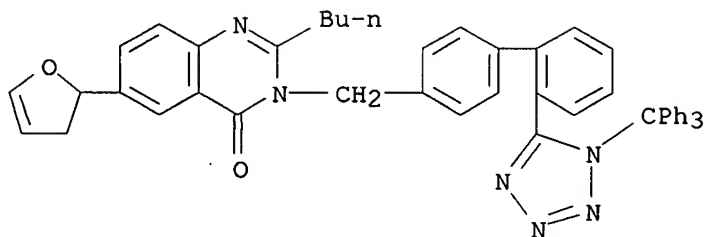
IT 158293-30-2P 158293-40-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

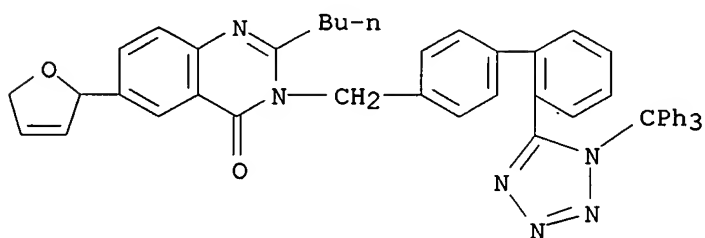
(preparation of, as intermediate for (furo[2,3-d]isoxazolyl)[(tetrazolyl)biphenyl]methyl]quinazolinone)

RN 158293-30-2 ZCAPLUS

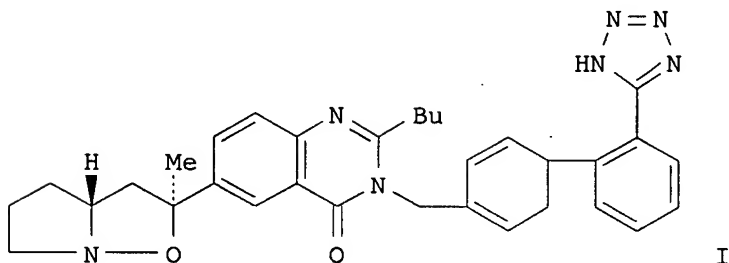
CN 4(3H)-Quinazolinone, 2-butyl-6-(2,3-dihydro-2-furanyl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



RN 158293-40-4 ZCAPLUS
 CN 4(3H)-Quinazolinone, 2-butyl-6-(2,5-dihydro-2-furanyl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI)
 (CA INDEX NAME)



L4 ANSWER 64 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:605279 ZCAPLUS
 DOCUMENT NUMBER: 121:205279
 TITLE: Synthesis and biological evaluation of the potent isoxazolidinyl angiotensin II receptor antagonist CL 332,877 and its enantiomers
 AUTHOR(S): Levin, Jeremy I.; Chan, Peter S.; Coupet, Joseph; Thibault, Lucien; Venkatesan, A. M.; Bailey, Trina K.; Vice, George; Cobuzzi, Agnes; Lai, Fong; Mellish, Noel
 CORPORATE SOURCE: Lederle Lab., American Cyanamide Co., Pearl River, NY, 10965, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(14), 1709-14
 CODEN: BMCLE8; ISSN: 0960-894X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB An alternative preparation of CL 332,877 (I), a potent (isoxazolidinyl)quinazolinone angiotensin II receptor antagonist, is

described. The enantiomers of CL332,877 were separated and evaluated both in vitro and in vivo.

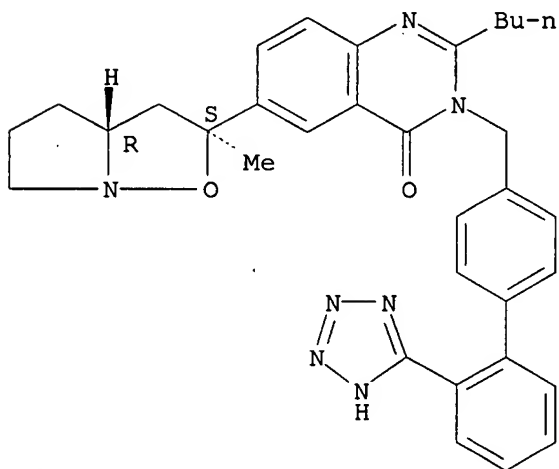
IT 157897-47-7P 157967-56-1P 157967-57-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antihypertensive CL 332,877)

RN 157897-47-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

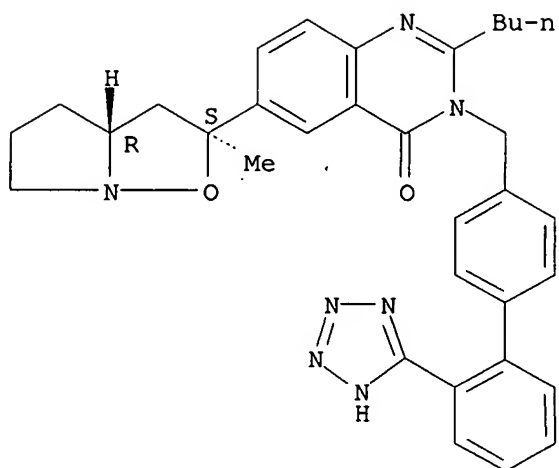


● Na

RN 157967-56-1 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, (2S-cis)- (9CI) (CA INDEX NAME)

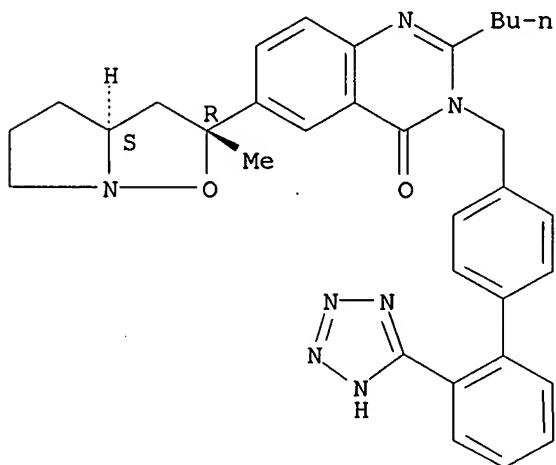
Absolute stereochemistry.



● Na

RN 157967-57-2 ZCAPLUS
 CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, sodium salt, (2R-cis)- (9CI) (CA INDEX NAME)

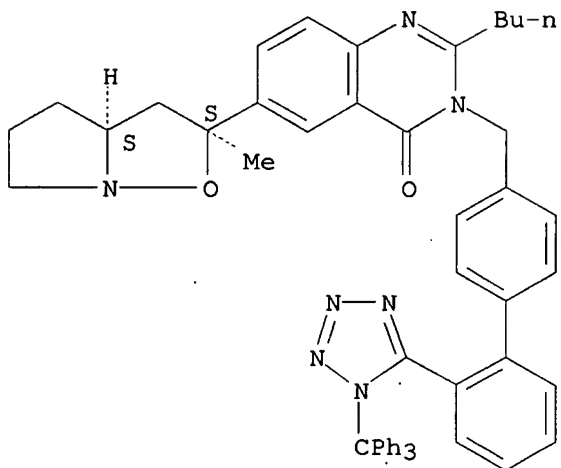
Absolute stereochemistry.



● Na

IT 155995-56-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as antihypertensive angiotensin antagonist)
 RN 155995-56-5 ZCAPLUS
 CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 157897-40-0P 157897-41-1P 157897-42-2P

157897-44-4P 157897-45-5P 157897-46-6P

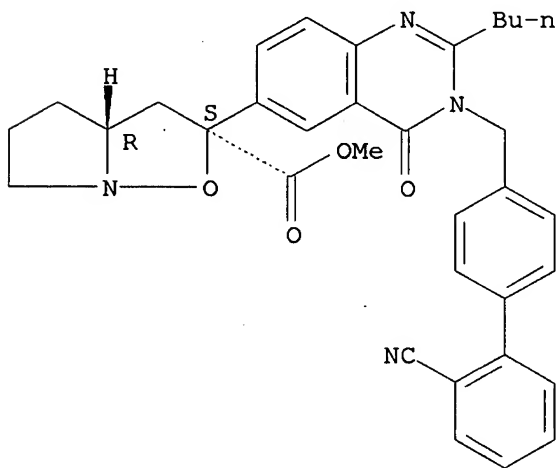
157967-54-9P 157967-55-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for CL 332,877)

RN 157897-40-0 ZCAPLUS

CN Pyrrolo[1,2-b]isoxazole-2-carboxylic acid, 2-[2-butyl-3-[(2'-cyano[1,1'-biphenyl]-4-yl)methyl]-3,4-dihydro-4-oxo-6-quinazolinyl]hexahydro-, methyl ester, trans- (9CI) (CA INDEX NAME)

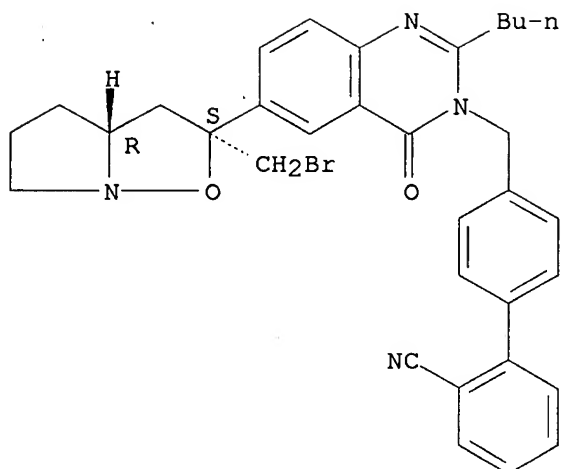
Relative stereochemistry.



RN 157897-41-1 ZCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[6-[2-(bromomethyl)hexahydropyrrolo[1,2-b]isoxazol-2-yl]-2-butyl-4-oxo-3(4H)-quinazolinyl]methyl]-, trans- (9CI)
(CA INDEX NAME)

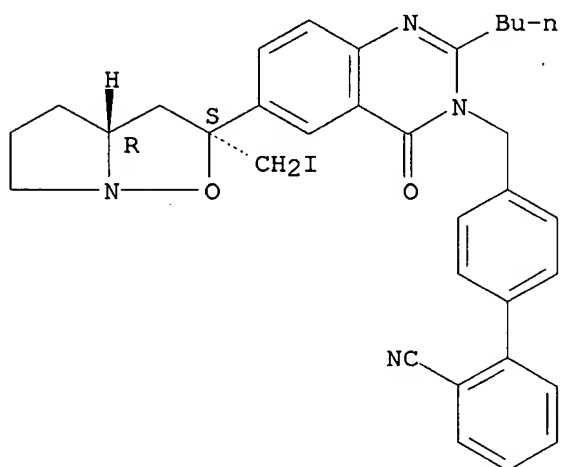
Relative stereochemistry.



RN 157897-42-2 ZCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[2-butyl-6-[hexahydro-2-(iodomethyl)pyrrolo[1,2-b]isoxazol-2-yl]-4-oxo-3(4H)-quinazolinyl)methyl]-, trans- (9CI) (CA INDEX NAME)

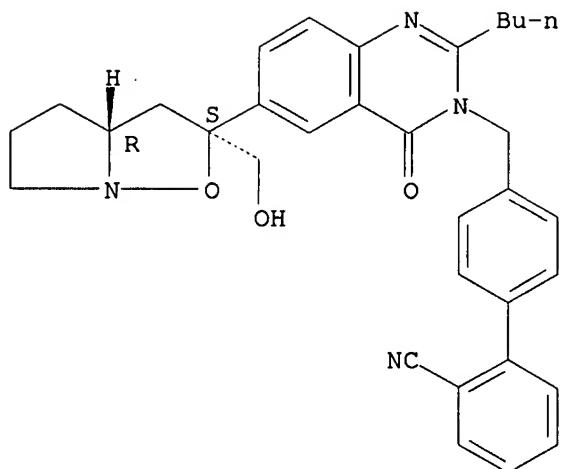
Relative stereochemistry.



RN 157897-44-4 ZCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[2-butyl-6-[hexahydro-2-(hydroxymethyl)pyrrolo[1,2-b]isoxazol-2-yl]-4-oxo-3(4H)-quinazolinyl)methyl]-, trans- (9CI) (CA INDEX NAME)

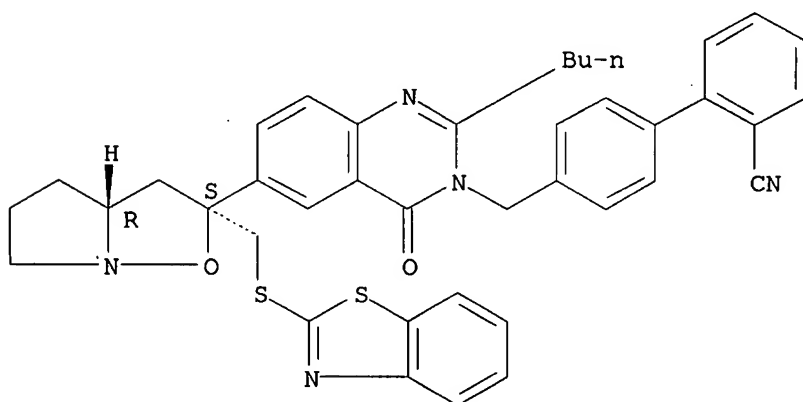
Relative stereochemistry.



RN 157897-45-5 ZCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[6-[2-[(2-benzothiazolylthio)methyl]hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl]-2-butyl-4-oxo-3(4H)-quinazolinyl]methyl]-, trans- (9CI) (CA INDEX NAME)

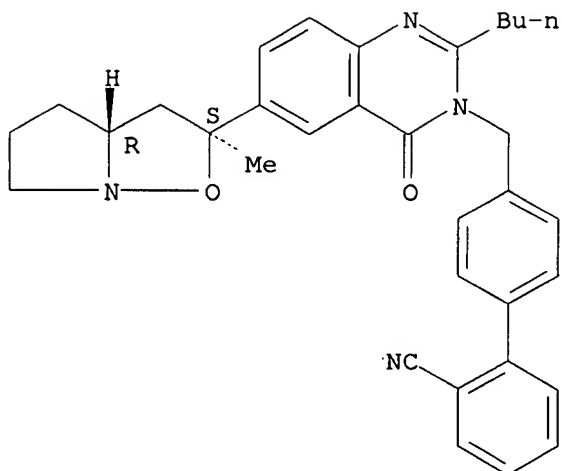
Relative stereochemistry.



RN 157897-46-6 ZCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-4-oxo-3(4H)-quinazolinyl]methyl]-, cis- (9CI) (CA INDEX NAME)

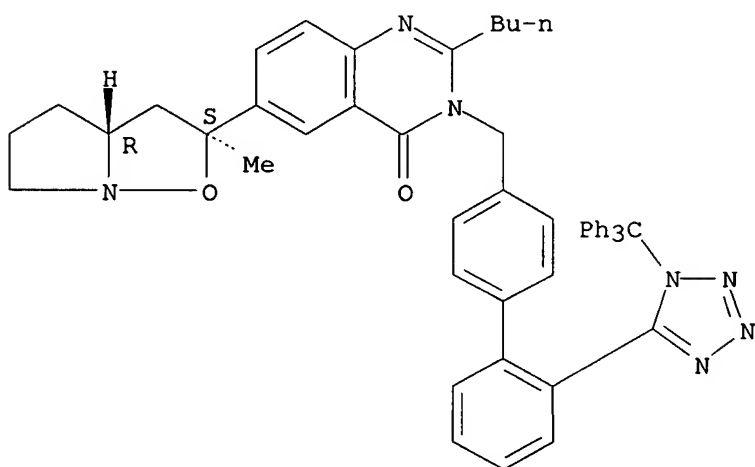
Relative stereochemistry.



RN 157967-54-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

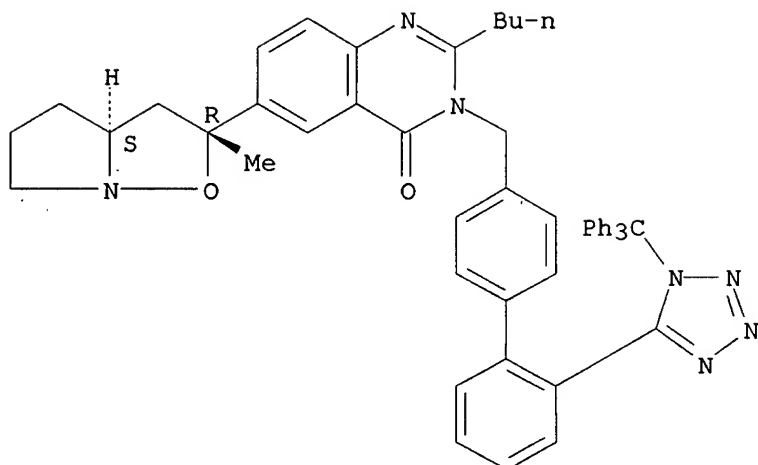
Absolute stereochemistry.



RN 157967-55-0 ZCAPLUS

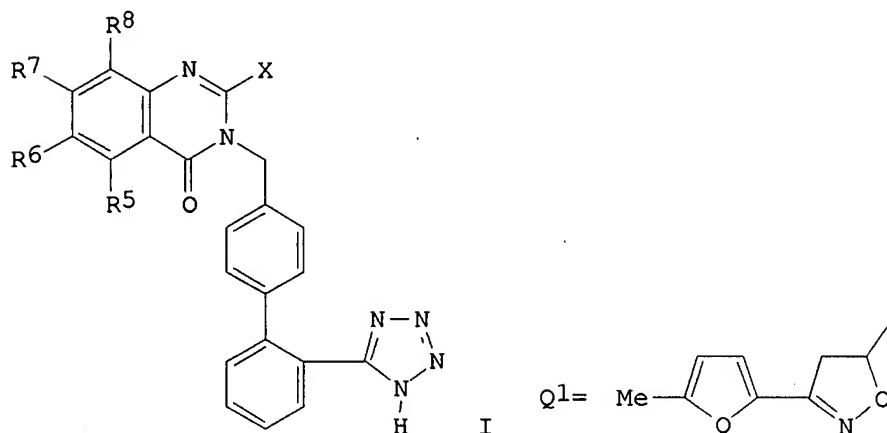
CN 4(3H)-Quinazolinone, 2-butyl-6-(hexahydro-2-methylpyrrolo[1,2-b]isoxazol-2-yl)-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 65 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:323587 ZCAPLUS
 DOCUMENT NUMBER: 120:323587
 TITLE: Angiotensin II receptor-blocking 2,3,6-substituted
 quinazolinones
 INVENTOR(S): Levin, Jeremy I.; Venkatesan, Aranapakam M.
 PATENT ASSIGNEE(S): American Cyanamid Co., USA
 SOURCE: U.S., 19 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5284853	A	19940208	US 1993-52943	19930423
PRIORITY APPLN. INFO.:			US 1993-52943	19930423
OTHER SOURCE(S):	MARPAT	120:323587		
GI				



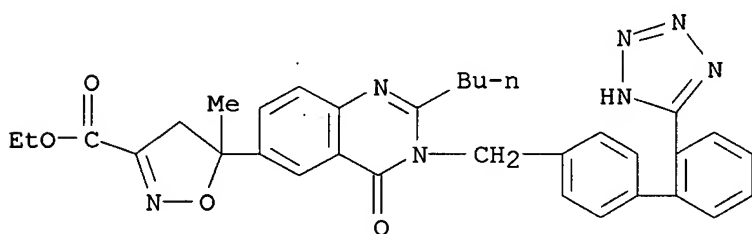
AB The title compds. [I; R5 = no definition given; R6 = (un)substituted dihydroisoxazolyl; R7, R8 = no definition given; X = (un)branched C3-5 alkyl], which are angiotensin II receptor antagonists useful for the treatment of hypertension and congestive heart failure (no data), are prepared Thus, quinazolinone I (R5 = R7 = R8 = H, R6 = Q1, X = Bu) was prepared and demonstrated beef adrenal gland-derived angiotensin II receptor 50% binding inhibition of 1.70×10^{-8} M.

IT 154749-08-3 154749-09-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(angiotensin II receptor antagonist)

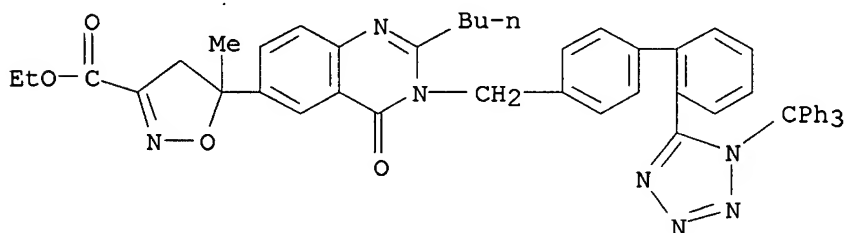
RN 154749-08-3 ZCAPLUS

CN 3-Isioxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 154749-09-4 ZCAPLUS

CN 3-Isioxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)



IT 154749-01-6P 154749-03-8P 154749-04-9P

154749-05-0P 154749-06-1P 154749-07-2P

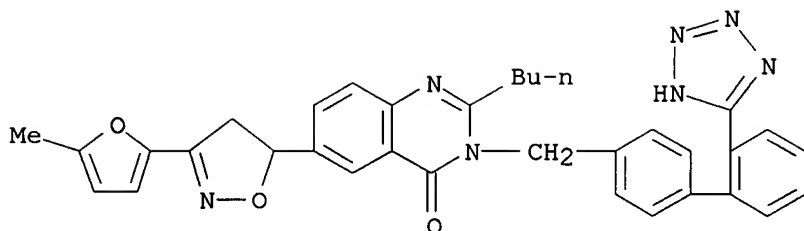
154749-10-7P 154749-11-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as angiotensin II receptor antagonist)

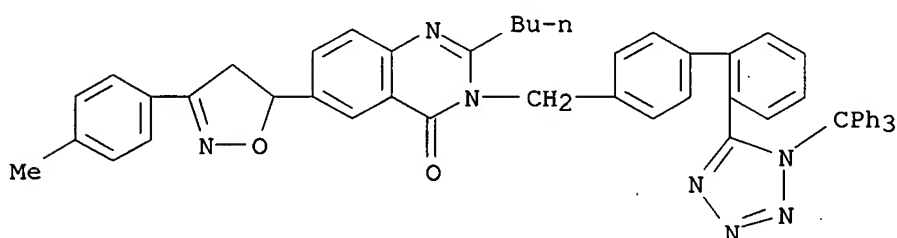
RN 154749-01-6 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(5-methyl-2-furanyl)-5-isioxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI)
(CA INDEX NAME)



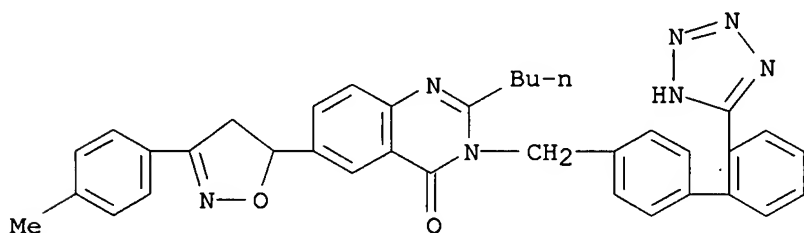
RN 154749-03-8 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methylphenyl)-5-isoxazolyl]-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



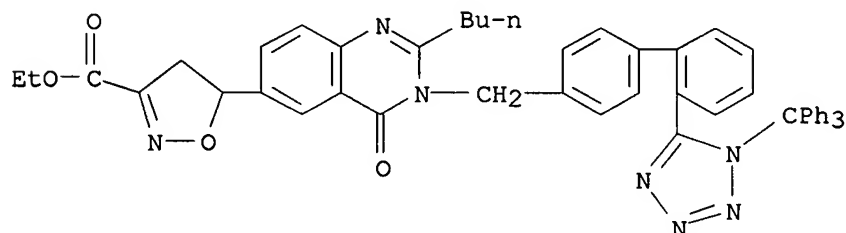
RN 154749-04-9 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(4-methylphenyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (CA INDEX NAME)



RN 154749-05-0 ZCAPLUS

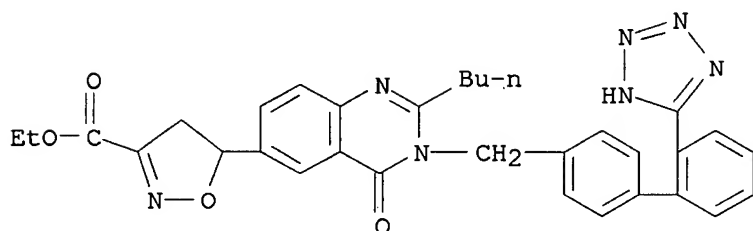
CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1-(triphenylmethyl)-1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-6-quinazolinyl]-4,5-dihydro-, ethyl ester (9CI) (CA INDEX NAME)



RN 154749-06-1 ZCAPLUS

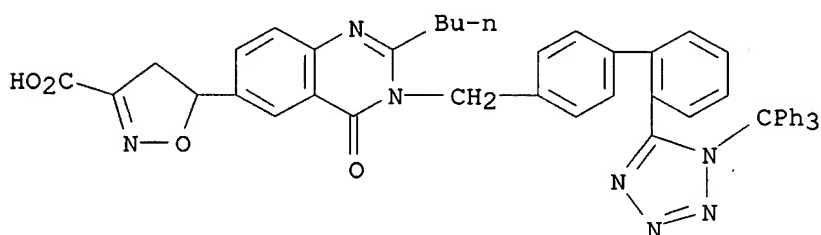
CN 3-Isoxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-

tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]-6-quinazolinyl]-4,5-dihydro-, ethyl ester (9CI) (CA INDEX NAME)



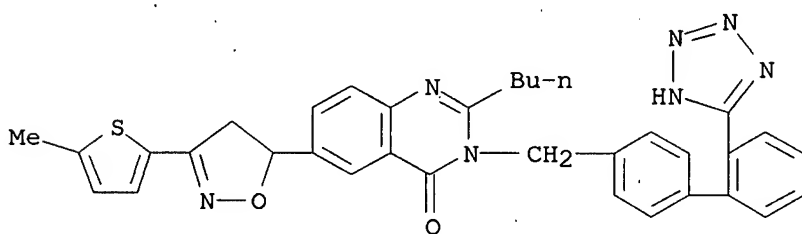
RN 154749-07-2 ZCAPLUS

CN 3-Isioxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]-6-quinazolinyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



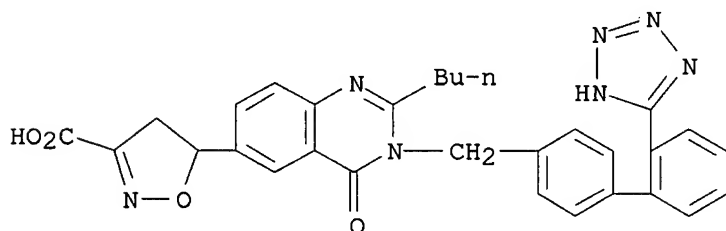
RN 154749-10-7 ZCAPLUS

CN 4(3H)-Quinazolinone, 2-butyl-6-[4,5-dihydro-3-(5-methyl-2-thienyl)-5-isoxazolyl]-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)

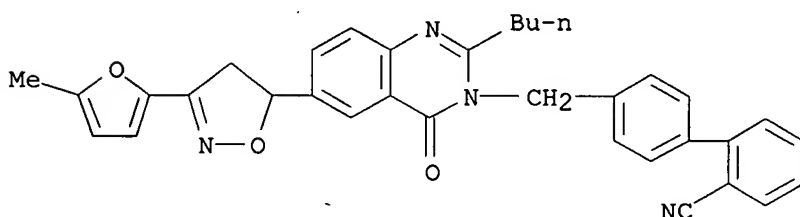


RN 154749-11-8 ZCAPLUS

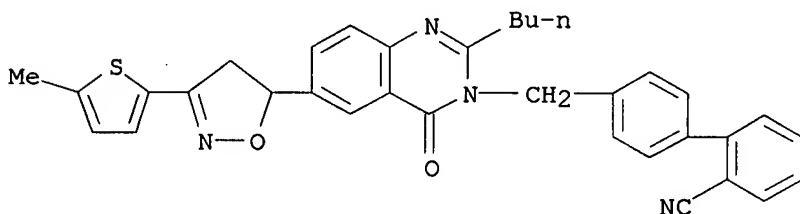
CN 3-Isioxazolecarboxylic acid, 5-[2-butyl-3,4-dihydro-4-oxo-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]-6-quinazolinyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



IT 154749-00-5P 154749-02-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, in preparation of substituted quinazolinone angiotensin II
 receptor antagonists)
 RN 154749-00-5 ZCAPLUS
 CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[2-butyl-6-[4,5-dihydro-3-(5-methyl-2-
 furanyl)-5-isoxazolyl]-4-oxo-3(4H)-quinazolinyl]methyl]- (9CI) (CA INDEX
 NAME)

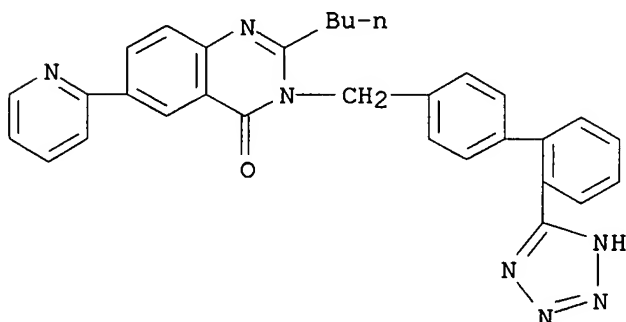


RN 154749-02-7 ZCAPLUS
 CN [1,1'-Biphenyl]-2-carbonitrile, 4'-[[2-butyl-6-[4,5-dihydro-3-(5-methyl-2-
 thienyl)-5-isoxazolyl]-4-oxo-3(4H)-quinazolinyl]methyl]- (9CI) (CA INDEX
 NAME)



L4 ANSWER 66 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:94722 ZCAPLUS
 DOCUMENT NUMBER: 120:94722
 TITLE: Quinazolinones. 2. QSAR and in vivo characterization
 of AT1 selective AII antagonists
 AUTHOR(S): de Laszlo, Stephen E.; Allen, Eric E.; Quagliato,
 Carol S.; Greenlee, William J.; Patchett, Arthur A.;
 Nachbar, Robert B.; Siegl, Peter K.; Chang, Raymond
 S.; Kivlighn, Salah D.; et al.
 CORPORATE SOURCE: Merck Res. Lab., Dep. Expl. Chem., Rahway, NJ, 07065,
 USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1993), 3(6),
 1299-304
 CODEN: BMCLE8; ISSN: 0960-894X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The structure activity relationship, linear regression anal. and in vivo
 evaluation of a series of substituted 2-butyl-3-[(2'-tetrazol-5-yl)biphen-
 4-ylmethyl]quinazolin-4(1H)-ones as antagonists of the AT1 receptor for
 angiotensin II is presented. L-159,093 (2-butyl-6-(N-isopropyl-N-methyl-
 carbamoyl)amino-3-[(2'-tetrazol-5-yl)biphen-4-ylmethyl]quinazolin-4(1H)-
 one) (IC50 = 0.1 nM rabbit aorta) is shown to be a potent orally active
 AII antagonist in rats and rhesus.

IT 152871-08-4
 RL: BIOL (Biological study)
 (angiotensin II AT1 antagonism by, structure in relation to)
 RN 152871-08-4 ZCAPLUS
 CN 4(3H)-Quinazolinone, 2-butyl-6-(2-pyridinyl)-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 67 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:603436 ZCAPLUS
 DOCUMENT NUMBER: 119:203436
 TITLE: Preparation of quinazolinones and pyridopyrimidinones useful as angiotensin II antagonists
 INVENTOR(S): Olson, Richard E.; Allen, Eric E.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: Eur. Pat. Appl., 66 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 534706	A1	19930331	EP 1992-308606	19920922
R: CH, DE, FR, GB, IT, LI, NL				
US 5202322	A	19930413	US 1991-765626	19910925
US 5256667	A	19931026	US 1992-923273	19920731
CA 2079079	A1	19930326	CA 1992-2079079	19920924
JP 06073024	A	19940315	JP 1992-254830	19920924
US 5308846	A	19940503	US 1993-96125	19930722
PRIORITY APPLN. INFO.:			US 1991-765626	A 19910925
			US 1992-923273	A 19920731
OTHER SOURCE(S):	MARPAT 119:203436			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [E = single bond, CHOH, CO, S(O)x(CH2)s, NR3(CH2)s; R3 = H, C2-4 alkanoyl, Ph, CH2Ph, C1-6 alkyl, C2-6 alkenyl, C3-7 cycloalkyl; s = 0-5; x = 0-2; G = (un)substituted Ph, carboxylate ester, CO2H, sulfonate ester, SO3H, etc.; R = aryl, heteroaryl, C3-7 cycloalkyl, H, alkynyl, alkenyl, (un)substituted alkyl, etc.; R2 = H, carbonylaryl, C3-7 cycloalkyl, halogen, OH, (un)substituted C alkyl, (un)substituted amino,

etc.; U, V, W = CH₂; N: provided there is only 1 N.; R₈, R₉ = (un)substituted C1-4 alkyl, halogen, OH, C1-5 alkoxy, H, CO₂H; X, Y = single bond, SO₂, O, (un)substituted CH₂, (un)substituted NH, etc.; Z = O, S(O)_x, (un)substituted NH, (un)substituted CH₂, useful for the treatment of hypertension (no data), are prepared Thus, quinazolinone II was prepared from quinazolinone III in 5 steps.

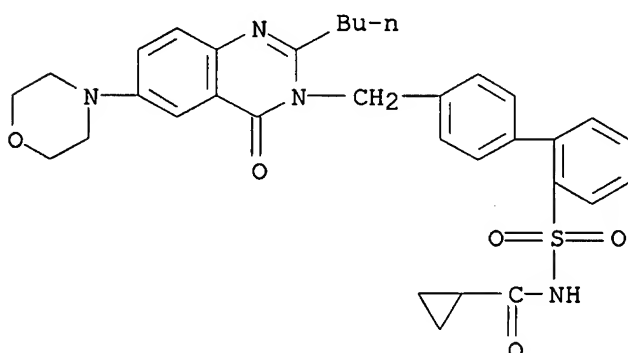
IT 150004-49-2P 150004-71-0P 150004-75-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and angiotensin II antagonist activity of)

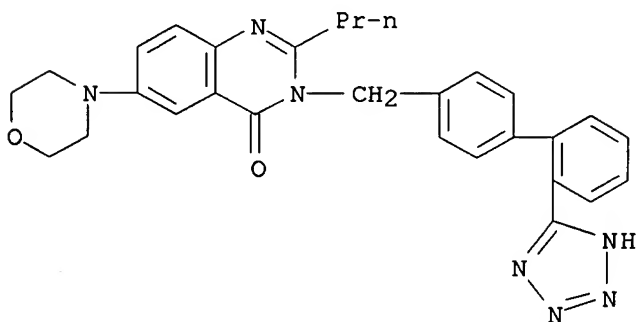
RN 150004-49-2 ZCAPLUS

CN Cyclopropanecarboxamide, N-[[4'-[[2-butyl-6-(4-morpholinyl)-4-oxo-3(4H)-quinazolinyl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)



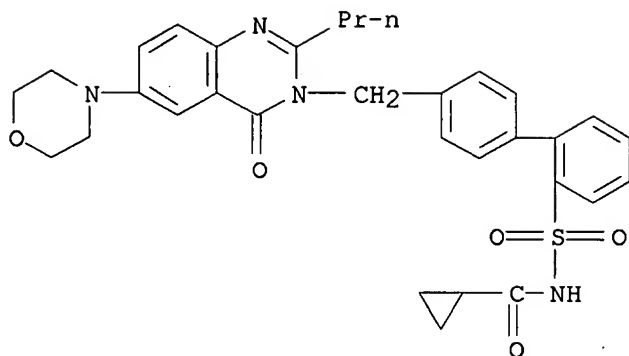
RN 150004-71-0 ZCAPLUS

CN 4(3H)-Quinazolinone, 6-(4-morpholinyl)-2-propyl-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

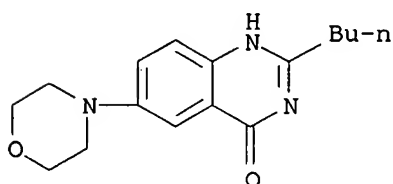


RN 150004-75-4 ZCAPLUS

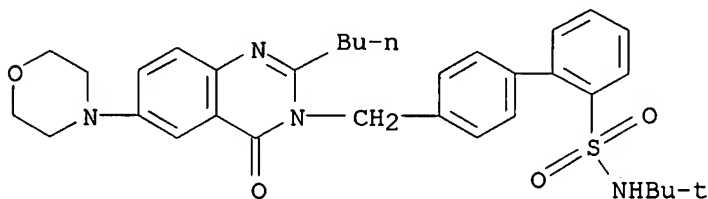
CN Cyclopropanecarboxamide, N-[[4'-[[6-(4-morpholinyl)-4-oxo-2-propyl-3(4H)-quinazolinyl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)



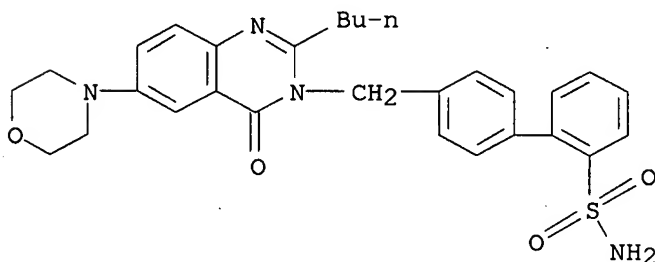
IT 150004-51-6P 150004-52-7P 150004-53-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, in preparation of angiotensin II antagonists)
 RN 150004-51-6 ZCAPLUS
 CN 4(1H)-Quinazolinone, 2-butyl-6-(4-morpholinyl)- (9CI) (CA INDEX NAME)



RN 150004-52-7 ZCAPLUS
 CN [1,1'-Biphenyl]-2-sulfonamide, 4'--[[2-butyl-6-(4-morpholinyl)-4-oxo-3(4H)-
 quinazolinyl]methyl]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

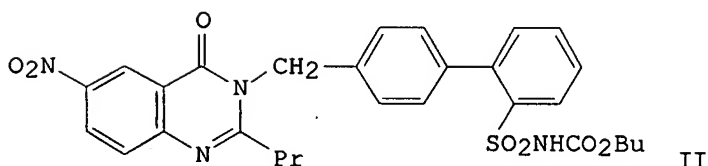
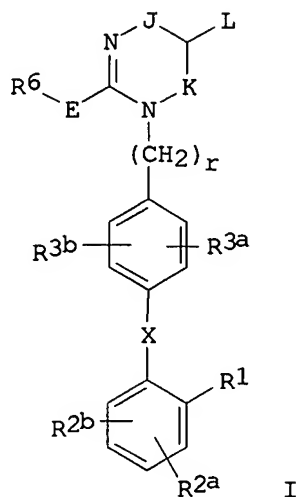


RN 150004-53-8 ZCAPLUS
 CN [1,1'-Biphenyl]-2-sulfonamide, 4'--[[2-butyl-6-(4-morpholinyl)-4-oxo-3(4H)-
 quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 68 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:169116 ZCAPLUS
 DOCUMENT NUMBER: 118:169116
 TITLE: Preparation of substituted quinazolinones as
 angiotensin II antagonists
 INVENTOR(S): Chakravarty, Prasun K.; Greenlee, William J.; Mantlo,
 Nathan B.; Patchett, Arthur A.; Dooseop, Kim; De
 Laszlo, Stephen E.; Glinka, Tomasz W.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: Eur. Pat. Appl., 119 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 512870	A1	19921111	EP 1992-304215	19920511
R: CH, DE, FR, GB, IT, LI, NL				
US 5238942	A	19930824	US 1992-867794	19920416
CA 2068229	A1	19921111	CA 1992-2068229	19920508
JP 05155867	A	19930622	JP 1992-117670	19920511
PRIORITY APPLN. INFO.:			US 1991-698506	A 19910510
			US 1992-867794	A 19920416
OTHER SOURCE(S):	MARPAT 118:169116			
GI				



AB Title compds. I [L is connected with J or K to form an aromatic ring as

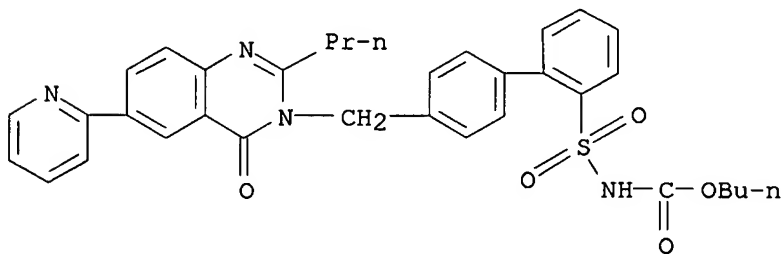
defined below; J = C:M or J and L are atoms to form a 6 membered (substituted) aromatic ring; K = C:M or K and L are connected to form a 6-membered (substituted) aromatic ring provided that only 1 of J and K is C:M; M = O, NR₂₂; R₁ = SO₂NR₂₅OR₂₅, SO₂NHSO₂R₂₃, SO₂NHCO₂R₂₃, etc.; R_{2a}, R_{2b} = H, halo, NO₂, NH₂, C₂-6 alkyl, CF₃, etc.; R_{3a} = H, halo, C₁-6 alkyl, C₁-6 alkoxy, C₁-6 alkoxyalkyl; R_{3b} = H, halo, NO₂, C₁-6 alkyl, C₁-6 acyloxy, C₃-7 cycloalkyl, C₁-6 alkoxy, etc.; E = bond, NR₁₃(CH₂)_sS(O)_x(CH₂)_s, CHOH, O, CO; x = 0-2; s = 0-5; R₆ = aryl, (substituted) C₁-6 alkyl, - C₂-5 alkenyl, - C₂-5 alkynyl, heteroaryl, C₃-7 cycloalkyl, perfluoro-C₁-4 alkyl, H; R₁₃ = H, C₂-5 alkanoyl, C₁-6 alkyl, allyl, C₃-6 cycloalkyl, aryl, arylmethyl; R₂₂ = aryl, heteroaryl, (substituted) C₁-4 alkyl; R₂₃ = aryl, heteroaryl, C₃-7 cycloalkyl, (substituted) C₁-6 alkyl, perfluoro-C₁-4 alkyl, diarylmethyl; R₂₅ = H, aryl, (substituted) C₁-6 alkyl; X = bond, CO, O, S, NR₁₃, OCH₂, CH₂O, SCH₂, CH₂S, CF:CH, etc.; r = 1, 2] were prepared as angiotensin II antagonists useful as antihypertensives (no data). Thus, 6-nitro-2-propyl-3-[(2'-(sulfonamido)biphenyl-4-yl)methyl]quinazolin-4-(3H)-one (preparation from 6-nitro-2-propylquinazolin-4(1H)-one and 4'-bromomethylbiphenyl-2-tert-butylsulfonamide given) in dry pyridine was treated with dimethylaminopyridine then ClCO₂Bu to give title compound II. Formulations containing I were prepared

IT 145863-75-8P 145863-76-9P 145863-78-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antihypertensive)

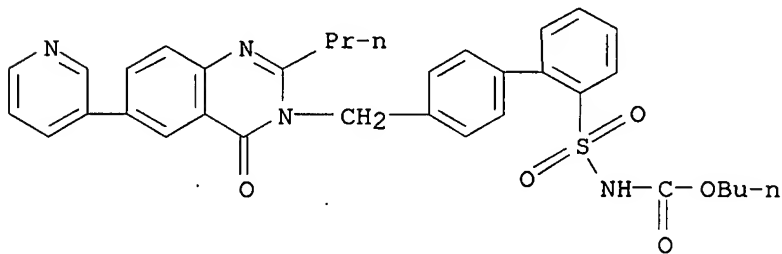
RN 145863-75-8 ZCAPLUS

CN Carbamic acid, [[4'-[[4-oxo-2-propyl-6-(2-pyridinyl)-3(4H)-quinazolinyl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]-, butyl ester (9CI)
(CA INDEX NAME)



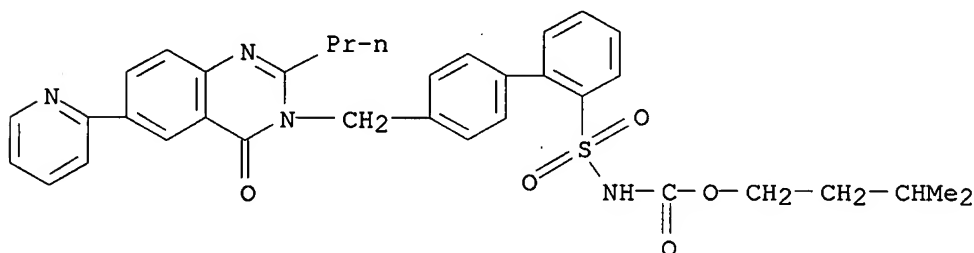
RN 145863-76-9 ZCAPLUS

CN Carbamic acid, [[4'-[[4-oxo-2-propyl-6-(3-pyridinyl)-3(4H)-quinazolinyl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]-, butyl ester (9CI)
(CA INDEX NAME)

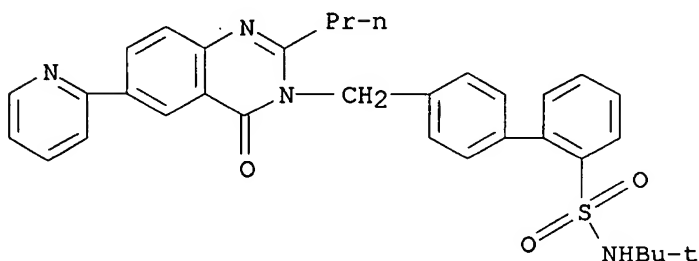


RN 145863-78-1 ZCAPLUS

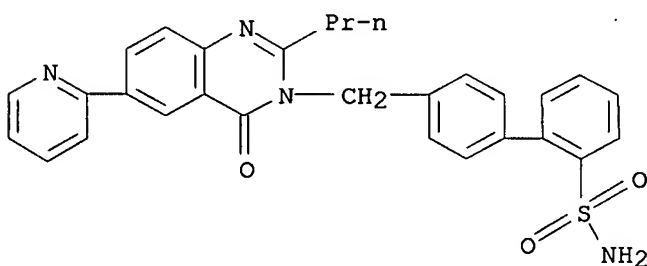
CN Carbamic acid, [[4'-[[4-oxo-2-propyl-6-(2-pyridinyl)-3(4H)-quinazolinyl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-, 3-methylbutyl ester (9CI) (CA INDEX NAME)



IT 145863-91-8P 145863-92-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for quinazolinone antihypertensives)
 RN 145863-91-8 ZCAPLUS
 CN [1,1'-Biphenyl]-2-sulfonamide, N-(1,1-dimethylethyl)-4'-[[4-oxo-2-propyl-6-(2-pyridinyl)-3(4H)-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)

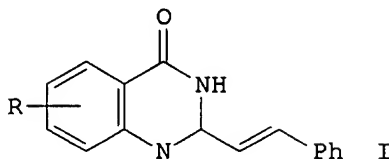


RN 145863-92-9 ZCAPLUS
 CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[[4-oxo-2-propyl-6-(2-pyridinyl)-3(4H)-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 69 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:235257 ZCAPLUS
 DOCUMENT NUMBER: 112:235257
 TITLE: Synthesis and biological evaluation of
 2-styrylquinazolin-4(3H)-ones, a new class of
 antimitotic anticancer agents which inhibit tubulin
 polymerization
 AUTHOR(S): Jiang, Jack B.; Hesson, D. P.; Dusak, B. A.; Dexter,
 D. L.; Kang, G. J.; Hamel, E.

CORPORATE SOURCE: E. I. Du Pont de Nemours and Co., Wilmington, DE,
19880, USA
SOURCE: Journal of Medicinal Chemistry (1990), 33(6), 1721-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:235257
GI



AB Title compds., e.g., I (R = 5-, 6-, 7-, 8-Cl, 6-Br, 6-F, 6-NH₂, 6-OMe, 5-, 6-Me, 6-OH, 6-OEt) were prepared. Extensive structure-activity relationship studies suggest that the entire quinazolinone structure was required, but activity was further enhanced by halide or small hydrophobic substituents at position 6. These analogs did not substantially interfere with the binding of radiolabeled colchicine, vinblastine, or GTP to tubulin and weakly stimulated GTP hydrolysis uncoupled from polymerization. Several analogs have shown in vivo tumor growth inhibitory activity in the L1210 leukemia model, with the lead compound I (R = 6-OMe) exhibiting good antitumor activity against murine solid tumors as well as human tumor xenografts.

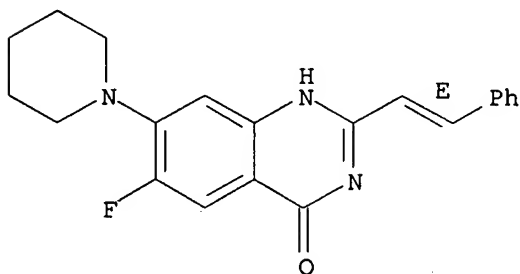
IT 127033-43-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)

RN 127033-43-6 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-fluoro-2-[(1E)-2-phenylethenyl]-7-(1-piperidinyl)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

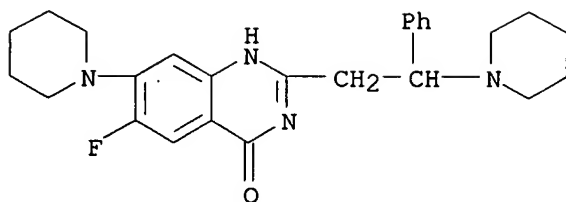


IT 127033-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and elimination of piperidine from)

RN 127033-53-8 ZCAPLUS

CN 4(1H)-Quinazolinone, 6-fluoro-2-[2-phenyl-2-(1-piperidinyl)ethyl]-7-(1-piperidinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 70 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:553834 ZCAPLUS

DOCUMENT NUMBER: 111:153834

TITLE: Preparation of benzoheterocycle derivatives as drugs for treating heart diseases

INVENTOR(S): Tamada, Shigeharu; Fujioka, Takafumi; Ogawa, Hidenori; Teramoto, Shuji; Kondo, Kazumi

PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

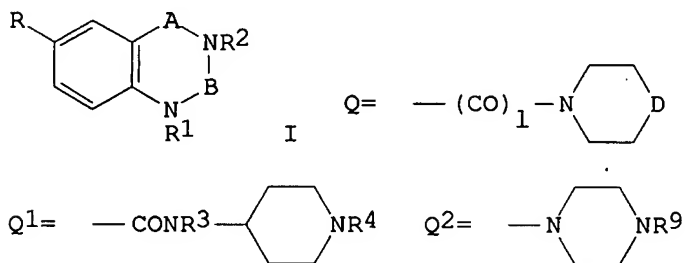
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01061468	A	19890308	JP 1987-218276	19870901
JP 2544939	B2	19961016		
PRIORITY APPLN. INFO.:			JP 1987-218276	19870901
OTHER SOURCE(S):	MARPAT	111:153834		

GI



AB The title compds. [I; R = H, Q, Q1, 1H-imidazo[4,5-c]pyridyl; R3 = H, lower alkyl; R4 = phenyl-lower alkyl having 1-3 substituents selected from lower alkoxy, halo, or NO₂ on Ph, phenylthio-lower alkyl, (N-lower alkyl) anilino-lower alkyl; 1 = 0, 1; D = CHNR5, NR7; R5 = H, lower alkyl, etc.; R7 = H, lower alkanoyl, etc.; R1 = H, lower alkyl, (halo)phenyl-lower alkyl, lower alkoxy-carbonyl-lower alkyl; R2 = H, lower alkyl, (halo) Ph; A = CH₂, CO, CR₈; R8 = H, Q2; R9 = H, phenyl-lower alkyl, (lower alkoxy) Bz; provided that when A = CR₈, R2 being unsubstituted and one of R and R8 = H; B = CO, CS, CR₁₀; R10 = H, lower alkyl, NH₂, pyridyl; provided that when B = CR₁₀, R1 being unsubstituted and A = CO] useful as cardiotonics, etc., were prepared A solution of 0.2 mL CCl₃O₂CCl in CH₂Cl₂ was added dropwise under ice-cooling to a solution of 2-aminomethyl-4-[4-(3,4-dimethoxybenzoyl)-1-piperazinyl]aniline 1.1 and Et₃N 0.8 g in 30 mL CH₂Cl₂ and the mixture was stirred 1 h under ice-cooling and 1 h at room temperature

After adding 5 N aqueous NaOH, the mixture was stirred overnight to give 0.35 g 6-[4-(3,4-dimethoxybenzoyl)-1-piperazinyl]-3,4-dihydro-2-quinazoline (II). I at 1 μ M, 100 or 300 nM increased 20-85.9% myocardial contractility and 0.5-3.0 mL/min coronary blood flow in dogs. A tablet (200 mg) containing II 5, starch 132, magnesium stearate 18, and lactose 45 mg was formulated.

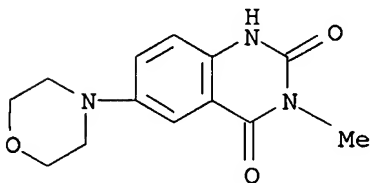
IT 122941-95-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with benzylamine, piperazinylquinazoline derivative from)

RN 122941-95-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-methyl-6-(4-morpholinyl)- (9CI) (CA INDEX NAME)



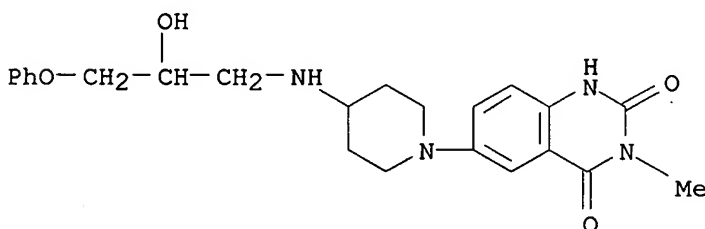
IT 122941-49-5P 122941-50-8P 122941-51-9P

122941-52-0P 122941-53-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cardi tonic)

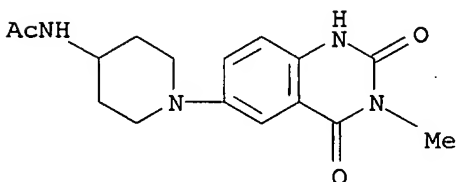
RN 122941-49-5 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-[4-[(2-hydroxy-3-phenoxypropyl)amino]-1-piperidinyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 122941-50-8 ZCAPLUS

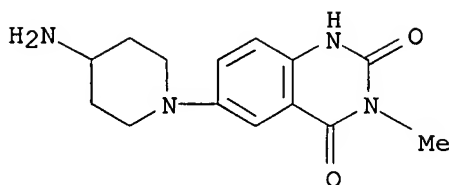
CN Acetamide, N-[1-(1,2,3,4-tetrahydro-3-methyl-2,4-dioxo-6-quinazolinyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)



RN 122941-51-9 ZCAPLUS

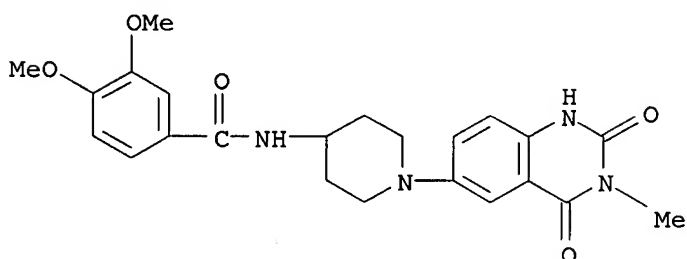
CN 2,4(1H,3H)-Quinazolinedione, 6-(4-amino-1-piperidinyl)-3-methyl- (9CI)

(CA INDEX NAME)



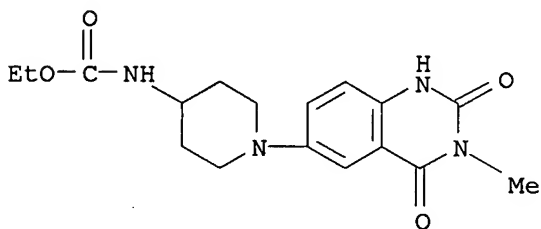
RN 122941-52-0 ZCAPLUS

CN Benzamide, 3,4-dimethoxy-N-[1-(1,2,3,4-tetrahydro-3-methyl-2,4-dioxo-6-quinazolinyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)



RN 122941-53-1 ZCAPLUS

CN Carbamic acid, [1-(1,2,3,4-tetrahydro-3-methyl-2,4-dioxo-6-quinazolinyl)-4-piperidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 71 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:62069 ZCAPLUS

DOCUMENT NUMBER: 104:62069

TITLE: 7-(1-Piperidinyl)-1,2,3,5-tetrahydroimidazo[2,1-b]quinazolin-2-one cancer metastasis inhibitor

INVENTOR(S): Ogawa, Hidemasa; Tanaka, Noriko

PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

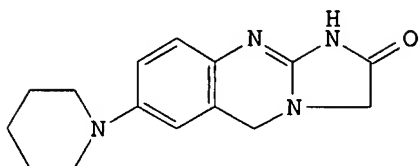
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60152416	A	19850810	JP 1984-7749	19840119

JP 03074206
 PRIORITY APPLN. INFO.:
 GI

B 19911126

JP 1984-7749

19840119



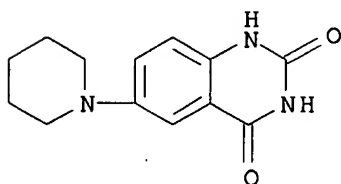
I

AB 7-(1-Piperidinyl)-1,2,3,5-tetrahydroimidazo[2,1-b]quinazolin-2-one (I) [96086-67-8] or its salt inhibits cancer metastasis. Thus, tumor B16BL6 (1 + 105 cells) injected i.v. into mice was metastasized, and the tumor was spread into the lung and killed all the control animals. However, oral administration of 10 mg I/kg prevented the mortality by 50%. I was prepared by treating 2-chloro-6-piperidino-3,4-dihydroquinazoline [96086-62-3] with Et bromoacetate [105-36-2], followed by an ammonium solution

IT 96086-60-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and chlorination of)

RN 96086-60-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 72 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:560469 ZCAPLUS

DOCUMENT NUMBER: 103:160469

TITLE: Cyclic guanidines. 17. Novel (N-substituted amino)imidazo[2,1-b]quinazolin-2-ones: water-soluble platelet aggregation inhibitors

AUTHOR(S): Ishikawa, Fumiyoshi; Saegusa, Junji; Inamura, Kazue; Sakuma, Kyoko; Ashida, Shinichiro

CORPORATE SOURCE: Res. Inst., Daiichi Seiyaku Co., Ltd., Tokyo, 134, Japan

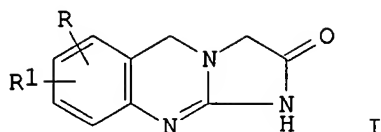
SOURCE: Journal of Medicinal Chemistry (1985), 28(10), 1387-93
 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:160469

GI



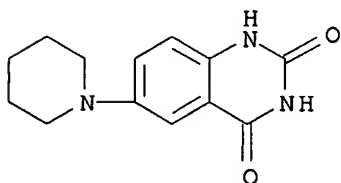
AB Aminotetrahydroimidazo[2,1-b]quinazolin-2-ones I [R = Me₂N, Et₂N, PhCH₂NMe, MeNH, pyrrolidino, morpholino, 4-methyl-1-piperazinyl, (un)substituted piperidino in 6-, 7-, or 8-position; R₁ = H, Cl] were prepared and were potent inhibitors of blood platelet aggregation in the rat. Some were H₂O-soluble and effective via i.v. infusion. Structure-activity relationships indicate that a lipophilic secondary amino group at position 6 or 7 contributed to retention of potent activity. I (R = 7-piperidino, R₁ = H) was the most effective, with an EC₅₀ of 0.33 μM in the in vitro test.

IT 96086-60-1P 96336-84-4P 97112-90-8P
97112-91-9P 97112-92-0P 97112-93-1P
97112-94-2P 97112-97-5P 97112-98-6P
97112-99-7P 97113-01-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination-aromatization of)

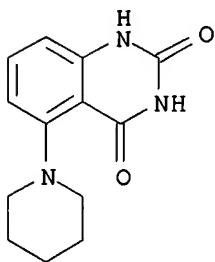
RN 96086-60-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



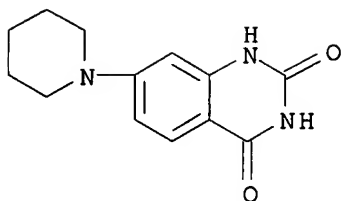
RN 96336-84-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5-(1-piperidinyl)- (9CI) (CA INDEX NAME)

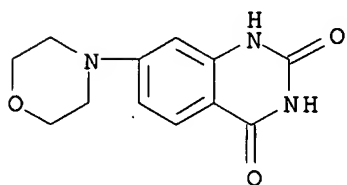


RN 97112-90-8 ZCAPLUS

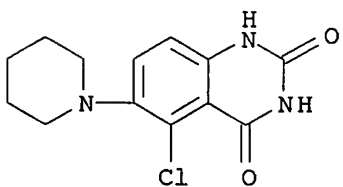
CN 2,4(1H,3H)-Quinazolinedione, 7-(1-piperidinyl)- (9CI) (CA INDEX NAME)



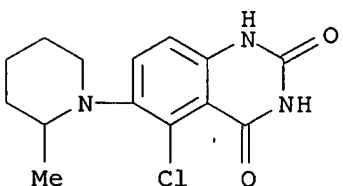
RN 97112-91-9 ZCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 7-(4-morpholinyl)- (9CI) (CA INDEX NAME)



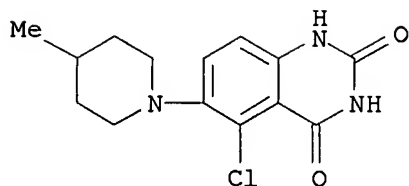
RN 97112-92-0 ZCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5-chloro-6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 97112-93-1 ZCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5-chloro-6-(2-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

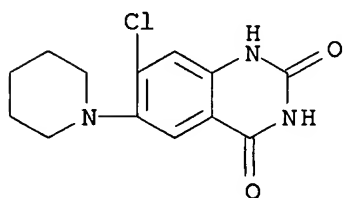


RN 97112-94-2 ZCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 5-chloro-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



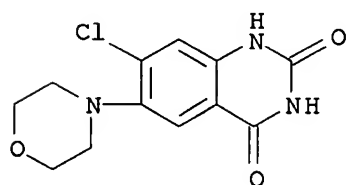
RN 97112-97-5 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-chloro-6-(1-piperidinyl)- (9CI) (CA INDEX NAME)



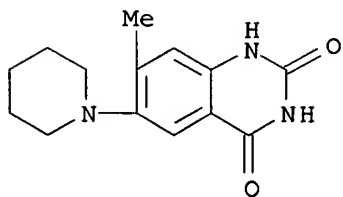
RN 97112-98-6 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-chloro-6-(4-morpholinyl)- (9CI) (CA INDEX NAME)



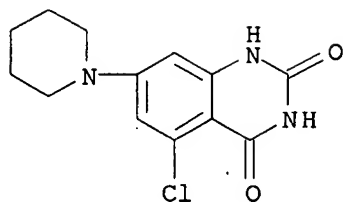
RN 97112-99-7 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 7-methyl-6-(1-piperidinyl)- (9CI) (CA INDEX NAME)

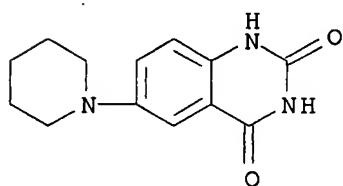


RN 97113-01-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5-chloro-7-(1-piperidinyl)- (9CI) (CA INDEX NAME)



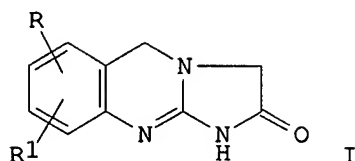
IT 97112-89-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 97112-89-5 ZCAPLUS
 CN 2,4(1H,3H)-Quinazolinedione, 6-(1-piperidinyl)-, monohydrochloride (9CI)
 (CA INDEX NAME)



● HCl

L4 ANSWER 73 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1985:203983 ZCAPLUS
 DOCUMENT NUMBER: 102:203983
 TITLE: Imidazoquinazolin-2-one compounds and pharmaceutical
 compositions containing them
 INVENTOR(S): Ishikawa, Fumiyoshi
 PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd. , Japan
 SOURCE: Eur. Pat. Appl., 50 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 133234	A2	19850220	EP 1984-108261	19840713
EP 133234	A3	19851030		
EP 133234	B1	19890412		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 60028979	A	19850214	JP 1983-128173	19830714
JP 04019996	B	19920331		
CA 1231947	A1	19880126	CA 1984-458566	19840710
US 4610987	A	19860909	US 1984-631417	19840716
PRIORITY APPLN. INFO.:			JP 1983-128173	A 19830714
OTHER SOURCE(S):	CASREACT 102:203983; MARPAT 102:203983			
GI				

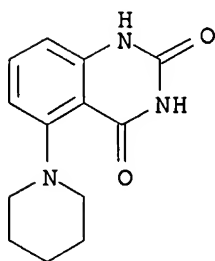


AB Title compds. I [R = dialkylamino, (un)substituted N heterocyclyl; R1 = H, halogen, alkyl, alkoxy] were prepared Thus, 2,5-O₂N(Cl)C₆H₃CN was aminated with Me₂NH to give the 5-Me₂N derivative which was reduced with NaBH₄ to give 5,2-Me₂N(O₂N)C₆H₃CH₂NH₂. The latter compound was treated with BrCH₂CO₂Et and catalytically reduced with 5% Pd-C to give 5,2-(Me₂N)(H₂N)C₆H₃CH₂NHCH₂CO₂Et which was cyclized with BrCN to give I (R = 7-Me₂N, R1 = H) (II). II inhibited ADP-induced aggregation of human platelets with an ED₅₀ of 7.2 μM and is accompanied by substantially no decrease in blood pressure and only a small increase in the heart rate.

IT 96336-84-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and chlorination of)

RN 96336-84-4 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 5-(1-piperidinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 74 OF 74 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:166773 ZCAPLUS

DOCUMENT NUMBER: 102:166773

TITLE: Imidazoquinazoline compound

INVENTOR(S): Ishikawa, Fumiyoshi; Ashida, Shinichiro

PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd. , Japan

SOURCE: Eur. Pat. Appl., 38 pp.
 CODEN: EPXXDW

DOCUMENT TYPE: Patent

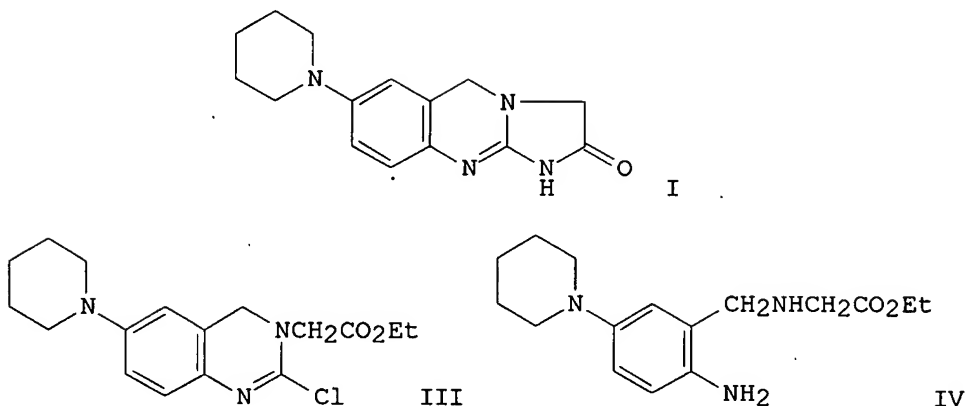
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 129258	A1	19841227	EP 1984-107130	19840620
EP 129258	B1	19870923		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 60004186	A	19850110	JP 1983-111498	19830621
JP 63005030	B	19880201		
ZA 8404437	A	19850130	ZA 1984-4437	19840612
DK 8402900	A	19841222	DK 1984-2900	19840613
DK 162999	B	19920106		

DK 162999	C	19920601		
CA 1231946	A1	19880126	CA 1984-456454	19840613
AU 8429432	A	19850103	AU 1984-29432	19840615
AU 558124	B2	19870122		
ES 533609	A1	19851216	ES 1984-533609	19840620
US 4596806	A	19860624	US 1984-622596	19840620
AT 29884	T	19871015	AT 1984-107130	19840620
FI 8402532	A	19841222	FI 1984-2532	19840621
FI 77864	B	19890131		
FI 77864	C	19890510		
NO 8402502	A	19841227	NO 1984-2502	19840621
NO 161220	B	19890410		
NO 161220	C	19890719		
IL 72188	A	19870331	IL 1984-72188	19840621
PRIORITY APPLN. INFO.:			JP 1983-111498	A 19830621
OTHER SOURCE(S):	CASREACT 102:166773		EP 1984-107130	A 19840620
GI				



AB 7-Piperidino-1,2,3,5-tetrahydroimidazo[2,1-b]quinazolin-2-one (I) was prepared by 2 methods. First, 2-chloro-6-piperidino-3,4-dihydroquinazoline, prepared in 5 steps from 5,2-Cl(O₂N)C₆H₃CN (II), was alkylated with BrCH₂CO₂Et to give quinazolineacetate III, which was treated with NH₃ at 120-130° for 4 h to give I. Second, piperidinobenzylaminoacetate IV, prepared in 4 steps from II, was treated with BrCN at room temperature to

give

I. I has not only potent platelet-aggregation inhibitory activity, but also inhibits metastasis of cancers, protects against stress-induced gastric ulceration, and stimulates secretion of pancreatic juice and bicarbonates.

IT 96086-60-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 96086-60-1 ZCAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 6-(1-piperidinyl)- (9CI) (CA INDEX NAME)